SPERC Background Document

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# Specific Environmental Release Categories (SpERCs) for the use of solvents and solvent-borne substances in the industrial production and/or use of explosives, synthetic rubbers, and blowing agents

## Introduction

Organic solvents comprise a large group of volatile substances that belong to one of three broad categories: hydrocarbon solvents, oxygenated solvents, and halogenated solvents. The commercial production of these substances takes place in closed reactors located at large petrochemical facilities that often operate adjacent to petroleum refineries supplying the raw feedstocks for their manufacture.

Solvents are used in a variety of industrial and commercial applications that harness their ability to act as extracting agents, solubilizers, cleansers or degreasers, and dispersing agents. Use of a solvent in a particular application is dictated, in part, by its physical and chemical properties, which can vary over a broad range. Solvents may also be used in combination when specific chemical characteristics are needed for a particular process or product.

Solvent emissions can take place during their production, storage, transport, and use. Air, water, and soil release are possible unless specific steps are taken to minimize or prevent the opportunity for unintentional discharge. These measures include the creation of specific operational controls that can be engineered into a product or process to limit environmental release and the potential for exposure. Examples include the use of containment devices, temperature control, and automated delivery systems. These control options are augmented by specific risk management measures (RMMs) that lessen the likelihood of release to a particular environmental compartment. RMMs can include any of a variety of pollution abatement technologies capable of capturing, neutralizing, or destroying a vapour, gas, or aerosol.

The following guidance document provides a description of the logic and reasoning used to create three Specific Environmental Release Categories (SpERCs). The air, water, and soil release factors associated with these SpERCs and sub-SpERCs provide an alternative to the default release factors associated with the environmental release categories (ERCs) promulgated by ECHA. The following sections of this background document have been aligned with those of the SpERC Factsheet and provide additional descriptive details on the genesis and informational resources used to generate each SpERC.

## 1. Title

The enclosed background information corresponds with the information provided in the following three factsheets:

1. ESVOC SPERC 2.18a.v3 – Use in explosives manufacturing
2. ESVOC SPERC 4.19a.v3 – Use in rubber production and processing
3. ESVOC SPERC 4.9.v2 – Use as blowing agents

Since these newly released SpERC factsheets include some corrections and or modifications, the version number has been changed to reflect the updates.

## 2. Scope

The applicability domain for a particular SpERC includes an initial determination of the life cycle stage (LCS) that best describes the industrial operation involved and the intended use of the substance being evaluated. The relevant life cycle stages and their interrelationships are depicted in Figure 1 (ECHA, 2015). The three SpERCs highlighted in this guidance document are all associated with a single life cycle stage: industrial end-use. This assignment is consistent with ECHA guidelines for distinguishing solvent uses in industrial applications versus their wide-spread use in professional or consumer applications.

Other use descriptors such as the sector of use (SU) and the chemical product category (PC) have been assigned in accordance with the naming conventions outlined by ECHA (ECHA, 2015). These have been summarized in Table 1 along with the use descriptions characterizing the three SpERCs. The terminology used to describe the individual applications is consistent with the list of standard phrases associated with the Generic Exposure Scenarios (GESs) that have been created to describe the exposures associated with the industrial production and use of solvents (ESIG/ESVOC, 2017). Use of standard phrases in these SpERC descriptions provides consistency and harmonization, and avoids confusion among potential SpERC users.

Figure 1. ECHA identified life cycle stages and their interrelationship

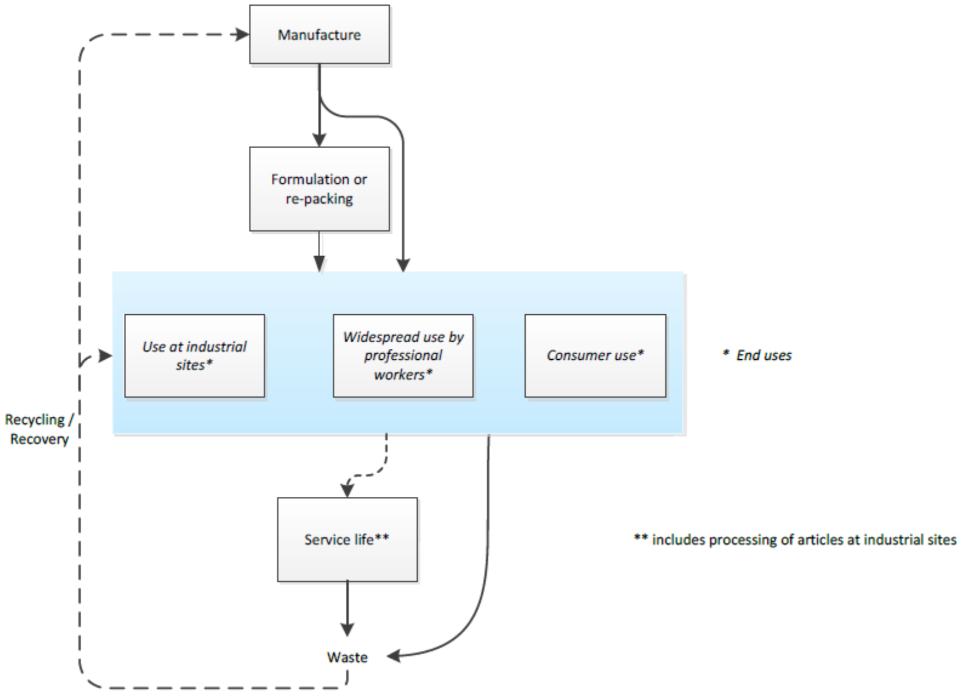

Table 1. SpERC background information

| SpERC Code | Title | Life Cycle Stage (LCS) | Sector of Use (SU) | Chemical Products Category (PC) | Use Description |
|---|---|---|---|---|---|
| ESVOC SPERC 2.18a.v3 | Use in explosives manufacturing | Industrial end-use | SU0 other | PC11 explosive | Covers exposures arising from the manufacture of slurry explosives (including materials transfer, mixing and charging) and equipment cleaning. |
| ESVOC SPERC 4.19a.v2 | Use in rubber production and processing | Industrial end-use | SU11 manufacture rubber products | PC0 other | Manufacture of tires and general rubber articles, including processing of raw (uncured) rubber, handling and mixing of rubber additives, vulcanising, cooling and finishing. |
| ESVOC SPERC 4.9.v2 | Use as blowing agents | Industrial end-use | SU18 Manufacture of furniture | PC32 polymer preparations and compounds | Use as a blowing agent for rigid and flexible foams, including material transfers, mixing and injection, curing, cutting, storage and packing |

## 3. Operational conditions

The operating conditions for a particular industrial application define a set of procedures and use conditions that limit the potential for environmental release. These system-related constraints are typically optimized to minimize emissions and maximize product yield within a particular manufacturing facility. Although the set of operating conditions applicable to a particular process are highly specific, some general details can be used to characterize the various production activities.**Conditions of use**

All three SpERCs are applicable to indoor industrial operations that manufacture or use the products in a controlled fashion that maximizes containment and minimizes opportunities for environmental release. This includes the use of appropriate storage containers, transfer devices, and minimization strategies for reducing product consumption. Open- and closed-loop batch reactors may also be relevant for operations where a wide range of specialty products are handled. In most cases, these operations do not use water as an extraction solvent, an adsorbent, or a reaction medium (OECD, 2011). The primary source of treatable wastewater results from the cleaning of drums, tanks, and transfer equipment. These wastewaters are subsequently treated at either an industrial or a municipal wastewater treatment (WWT) plant.

Evidence suggests, however, that municipal WWT plants are not widely used to process industrial wastewaters. This is supported by several surveys of industrial wastewater treatment at European facilities. The first involved a survey of WWT technologies at 81 European chemical facilities that included both large integrated facilities and smaller dedicated stand-alone sites (EC, 2016). The operations at these facilities included the production and formulation of a wide range of chemicals and solvents for use in a wide range of downstream applications. The survey results indicated that a majority (i.e. 89%) of the chemical facilities used a dedicated industrial wastewater treatment facility; a much smaller percentage utilized a municipal treatment plant capable of handling both industrial and domestic wastewater. The second survey of industrial operations in Germany found that 4% of the wastewater generated was directed to municipal WWT plants (DECHEMA, 2017). Despite the limited reliance on municipal treatment facilities, their usage is conservatively assumed to exist as a normal operating condition during the downstream use of solvents in industrial operations.

Rigorous containment is not a necessary prerequisite for the application of these SpERCs to an environmental exposure analysis. The European Chemical Agency has outlined the technical and operational requirements necessary to demonstrate that a volatile organic compound (VOC) has been rigorously contained. These include but are not limited to a variety of control measures that minimize the release of a volatile solvent during processing or handling (ECHA, 2010). Strict emission control is not a necessary prerequisite for the use of these SpERCs in the described applications.

### 3.2. Waste handling and disposal

Every effort should be made to minimize the generation of waste solvents at every stage of the life cycle. This includes the implementation of sensible waste minimization practices that stress the importance of recycling and/or reuse. Under most circumstances, the residual waste generated during the industrial use of a solvent-containing product is handled as a liquid or solid hazardous waste (EEA, 2016). This designation applies to each of the SpERCs described herein and implies the implementation of specific risk management measures to ensure proper storage, transport, and disposal of the waste. These include a detailed written description of the physical form, industrial source, and chemical composition of the waste; the use of continually monitored dedicated storage bunkers or tanks for quarantining the waste; and the maintenance of up to date records documenting the handling and disposal methods (EA, 2004). The residual hazardous waste may be disposed of through thermal incineration using any of several high efficiency equipment designs including rotary kilns (EC, 2017).

## 4. Obligatory risk management measures onsite

Application of the described SpERCs is not dependent on the implementation of obligatory RMMs to control atmospheric release during production or processing. It is assumed, however, that all applicable industrial operations include intensive and detailed housekeeping practices that help minimize environmental release. In addition, biological wastewater treatment is an obligatory risk management measure that ensures the biodegradation of any water-soluble volatile substance prior to discharge in a local waterway. It is also supposed that all immiscible liquids have been removed from the wastewater influent using an acceptable oil-water separator or dissolved gas flotation device. Finally, onsite or offsite hazardous waste destruction of any unrecovered solvents is a necessary waste management practice (ECHA, 2012).

These required measures can be supplemented with any of several optional control devices that can further reduce environmental emissions. When implemented, the effectiveness of these measures may be used to reduce the release factors associated with the applicable sub-SpERC.

### 4.1. Optional risk management measures limiting release to air

The following optional RMMs may be applicable to some or all of the SpERCs highlighted in this guidance document. If relevant, the stated air release factors may be adjusted downward to account for the additional reductions in environmental emission. Seven treatment technologies have been cited in Table 2 along with the range of measured removal efficiencies, the assigned nominal removal efficiency for use when adjusting the assigned air emission factor, and the SpERCs where the technology may be applicable.

The treatment technologies include wet scrubbers, thermal oxidation, vapour adsorption, membrane separation, biofiltration, cold oxidation, and air filtration (EC, 2016, Schenk, et al., 2009). The removal efficiency of wet scrubbers for VOCs can vary depending on the plant configuration, equipment operating conditions, and the type of VOC. The range of removal efficiencies cited in Table 2 reflect the variability that has been observed in three separate determinations. Two of these determinations found a removal efficiency of 70% or greater, whereas a third reported a range of 50 - 95%. The latter measurements included the use of a fibrous bed scrubber which is best suited for use with particulates. Taking these facts into consideration, a conservative default value of 70% was judged to be representative of the removal efficiency of wet scrubbers for solvent volatiles.

Table 2. Treatment technologies and removal efficiencies for reducing the air emission factors for VOCs

| Air abatement technology | Reported abatement efficiency range (%) | Assigned abatement efficiency (%) | Applicability to individual SpERCs | | |
|---|---|---|---|---|---|
| | | | ESVOC SPERC 2.18a.v3 | ESVOC SPERC 4.19a.v3 | ESVOC SPERC 4.9.v2 |
| wet scrubbers | 50 - 99 | 70 | X | X | Z |
| thermal oxidation | 95 - 99.9 | 95 | X | X | X |
| solid adsorbent | 80 - 95 | 80 | X | X | Z |
| membrane separation | <99 | 80 | Z | Z | Z |
| biofiltration | 75 - 95 | 75 | Z | Z | Z |
| cold oxidation | 80 - >99.9 | 80 | Z | Z | Z |
| air filtration | 70 - 99 | 70 | Z | X | Z |

X – abatement technology broadly applicable
Z – abatement technology may be applicable

The abatement efficiency of thermal oxidizers was found to range from 95 - 99% in one study and 98 - 99.9% in another. A conservative default value of 95% was established at the low end of the distribution to ensure that an adequate margin of safety had been incorporated into any emission factor adjustment. The use of solid adsorbents such as granular activated carbon, zeolite, or macroporous polymers offered capture efficiencies ranging from 80 - 99% in three separate studies. A nominal default value of 80% was determined to provide adequate assurance that the removal efficiency for this technology was not overestimated. Membrane separation techniques allow for the selective recovery of a volatile substance and can yield a range of efficiencies up to 99% depending on flow rates, properties of the substance, and membrane type. A nominal removal efficiency of 80% was assigned to this technology to ensure that an adequate margin of protection is included in any emission factor adjustments.

Removal efficiencies ranging from 75 - 95% have been observed when biofilters are used as an emission abatement technology for volatile substances. The variance is due in part to the wide range of biological materials that can be used to construct the filtration bed (e.g. peat, compost, tree bark, and softwoods). To account for the variability and ensure adequate caution, a nominal removal efficiency of 75% should be applied when this technology is in use. Cold oxidation methods for emission abatement include systems capable of ionizing and oxidizing a vapour through the application of a strong electric current. Differences in equipment design and operational conditions can affect the removal efficiencies observed using this approach. The nominal removal efficiency of a volatile substance by cold oxidation has been set at the lower end of the observed range of 80 - >99%. Higher removal efficiencies may be applied when any of these technologies are used in combination within a vapor recovery unit. Air filtration techniques such as wet dust scrubbing may be used to remove soluble particulate matter, aerosols, and mist from an airstream. The removal efficiencies attainable with these methods varies depending the type of scrubber being used, with reductions of 70 - 99% observed with a fibrous packing scrubber using glass, plastic, or steel packing material.

The preceding list of air treatment technologies is not exhaustive; others may exist that are capable of capturing volatiles and ameliorating the air emission profile. These include technologies such as cryo-condensation, bio-trickle filtration, and bio-scrubbing. If they apply, the abatement efficiencies for these emission control devices can be retrieved from either of several different literature sources (EC, 2016, Schenk, et al., 2009).**Optional risk management measures limiting release to water**

The SPERC release factors assume that there is no undissolved material in the wastewater stream being biologically degraded. If this is not the case then the immiscible liquids need to be removed using either of several separation techniques. These include the use of oil-water separators or dissolved gas flotation devices. Oil-water separators employing a skimming device for oil removal have been shown to operate with an abatement efficiency of 80 - 95% depending on the equipment design, the amount of immiscible material in the wastewater, and the physical characteristics of the recoverable material (EC, 2016). Most equipment designs incorporate i) parallel plate or corrugated plate interceptors or ii) the American Petroleum Institute (API) mechanical separator.

Dissolved gas flotation devices use pressurized gas treatment to generate small gas bubbles that capture any suspended oil. The removal efficiency using this treatment technology can vary from 50 - 90% depending the specific characteristics of the wastewater stream (Galil and Wolf, 2001). Flocculants may be added to the wastewater stream to improve coagulation and entrapment of the emulsified oil.

### 4.3. Optional risk management measures limiting release to soil

The emission factors are only applicable to facilities and operations were there is no application of WTP sludge to agricultural soil or arable land (ECHA, 2016). It also understood that good housekeeping and maintenance procedures are in place to minimize the potential for soil release. Aside from these requirements, there are no discretionary risk management measures that may be instituted to minimize the release of volatile substances to soil (CEFIC, 2007).

## 5. Exposure assessment input

The exposure scenarios used to evaluate the potential risk from the environmental release of a substance are highly dependent on the identification of certain key parameters that allow the air, water, and soil concentrations to be predicted. Factors such as the use rate, emission duration, and environmental release magnitude need to be quantified and substantiated in a manner that provides credence to final risk determination. This section of the background document describes the approach, reasoning, and information resources used to establish a reasonably conservative value for these key parameters.

### 5.1. Substance use rate

The three SpERCs identified in this guidance document have slightly dissimilar maximum estimated usage rates that reflect differences in the handling capacities at different industrial sites (see Table 3). The maximum site tonnages have been established using expert sector knowledge along with published information that provides representative nameplate capacities at typical site operations. The stated values provide a realistic worst-case estimate of the usage per day and may be modified if i) more realistic data is available; ii) the use amount needs to be limited to manage the environmental risk; and iii) the number of emission days is less than the cited value. The local or regional fractional use tonnages are generally adjusted for the wide dispersive uses that accompany professional and consumer applications, so there has not been any modification for the industrial applications described in these three SpERCs.

Table 3. Maximum estimated rates of usage and the fractional tonnages used at the local and regional level

| **Tonnage** | **SpERC title** | | |
|---|---|---|---|
| | **ESVOC SPERC 2.18a.v3** | **ESVOC SPERC 4.19a.v3** | **ESVOC SPERC 4.9.v2** |
| Local use rate (kg/day) | 50,000 | 100,000 | 50,000 |
| Emission days | 300 | 300 | 300 |
| Fractional local EU tonnage | 100% | 100% | 100% |
| Fractional regional EU tonnage | 100% | 100% | 100% |
| Rationale | tanker truck shipments | published citation | tanker truck shipments |

The estimated local use rate at sites manufacturing explosives and blowing agents was based on professional judgement and take into consideration the number of tanker trucks that are off-loaded at a representative facility per day. These tankers are assumed to operate in accordance with EU Directive 96/53/EC governing the maximum authorized weights and dimensions of road trailers in Europe (EU, 1996). In agreement with the legislation, the payload capacity of the transport vehicles is presumed to be 25 metric tons (Znidaric, 2015). The number of off-loaded tanker trucks processed at a site was conservatively estimated to be 2 per day for explosives manufacturing and for use as a blowing agent. The equation used to calculate the use rates is as follows:

$$Use\ rate\ \left(\frac{kg}{day}\right) = tanker\ payload\ (tonnes) \times loading\ frequency\ \left(\frac{tankers}{day}\right) \times 1000\ \left(\frac{kg}{tonne}\right) \qquad (1)$$

The local use rate for the rubber manufacturing SpERC was estimated using published information on production volume of synthetic rubbers in the European Union (Rubber-Economist, 2009). An evaluation of synthetic rubber production capacity in 12 EU countries reported a 2008 volume of 2.5 million tonnes. This volume was projected to decline by about 17% over the next three years. This 2008 value equates to 208,000 tonnes per region or 20,800 tons per manufacturing site, assuming that there are at least 10 manufacturing operations per region. Based on this analysis, the use rate per site was conservatively assumed to be no greater than 300,000 tonnes/year or 100,000 kg/day for a 300-day production cycle. The equation used to calculate the overall use rate is as follows:

$$Use\ rate\ \left(\frac{kg}{day}\right) = \frac{plant\ capacity\ \left(\frac{tonnes}{year}\right) \times 1000\ \left(\frac{kg}{tonne}\right)}{operating\ period\ \left(\frac{days}{year}\right)} \qquad (1)$$

The preceding determinations provide a conservative estimate of the of the use rate that can be expected at production and use facilities in Europe.

### 5.2. Days emitting

The number of emission days is the same for each of the SpERCs described in this guidance document (see Table 3). The value of 300 days/year is the default value for substances used in industrial applications in an amount greater than 5,000 tonnes/year (ECHA, 2016). The tonnage cut-off limits cited above represent the maximum use amount at a single site.

### 5.3. Release factors

The magnitude of an environmental emission following the production or use of a volatile solvent may be impacted by its water solubility and volatility (OECD, 2011). Since these properties can vary over a wide range for the bulk commodity solvents found in commerce, a single emission factor does not adequately portray the release of all the chemicals in this class. This has prompted the identification of individual emission factors that reflect the differences in the physical and chemical properties of a volatile substance. Numerical classification allows solvents with high water solubility or volatility to be distinguished from those with a low to intermediate values. Using this approach, a single vapor pressure category was used along five water solubility categories to define five sub-SpERCs for each identified use. This yielded a more precise scheme for assigning a release factor to a volatile solvent with particular water solubility characteristics.

#### *a) Release factor to air*

A failure to locate suitable information across a range of vapor pressure categories necessitated a pragmatic assignment of air release factors. When reliable information was unavailable for the solvents used in a particular industrial application, a worst-case default estimate was applied. Otherwise, published air release factors were applied once the information was suitably vetted. Table 5 provides a listing of the emission factors and their associated literature sources for each of the three SpERCs being considered.

Table 5. SpERC release factors for air

| **Assignments** | **SpERC title** | | |
|---|---|---|---|
| | **explosive use** | **rubber processing** | **blowing agent use** |
| Air release factor (%) | 0.5 | 1.0 | 98 |
| Source | (Hägvall, et al., 2004) | (OECD, 2004) | (ECHA, 2016) |

1. Use in explosives

A life cycle assessment (LCA) for the production and use of a pre-fragmented high explosive (PFHE) grenade included an examination of the air emissions resulting from the production of several explosive chemicals (Hägvall, et al., 2004). The air release of NMVOCs associated with the manufacture of ammonium nitrate (AN) and trinitrotoluene (TNT) were reported to be 0.44 kg/tonne and 0.71 kg/tonne of product, respectively. These values are equivalent to NMVOC air emission factors of 0.04% for AN and 0.07% for TNT. Unlike AN, TNT production was also associated with the atmospheric release of 4.62 kg/tonne of toluene. After summing the releases of NMVOCs and toluene, a total air release factor of 5.3 kg/tonne or 0.5% was obtained for TNT. This value provides a well substantiated and suitably conservative assessment of organic vapour emissions associated with the manufacture of explosives.

2. Use in rubber production and processing

The air release factor for synthetic rubber production has been taken from an analysis performed in the OECD Emission Scenario Document (ESD) for the rubber industry (OECD, 2004). The value of 1.0% is applicable to polymer industry processing aids with a vapour pressure greater than 100 Pa and a boiling point less than 300 °C. The OECD assigned air emission factor was associated with the Appendix I A-Table value assigned to substances used in the polymer industry (EC, 2003).

3. Use as blowing agents

The ERC 4 default value of 98% has been adopted since factual information describing the actual air emission value is unavailable (ECHA, 2016). The listed default value has been attributed to the use of non-reactive processing aids at an industrial site (no inclusion into or onto article). Processing aids include the use of solvents in continuous or batch processes using dedicated or multi-purpose equipment that is either automatically or manually controlled. The genesis of this value reportedly stems from an examination of the release factors posted in the A-Tables of Appendix 1 in the Technical Guidance Document (TGD) on Risk Assessment PART II (EC, 2003).

The air emission factors shown in Table 5 have not been adjusted for the potential use of an emission abatement device such as those described in section 4.1. Using fractional values, the adjustment is easily calculated using the following formula:

$$Adjusted\ release\ factor = unadjusted\ release\ factor \times (1 - abatement\ removal\ efficiency) \qquad (3)$$

The use of an adjusted air emission factor in a SpERC application must be fully documented and explained in the Chemical Safety Report.

***b) Release factor to water***

The fractional release of a volatile substance into the wastewater stream can be calculated as the ratio of the released mass to the overall production mass. The mass of a volatile solvent released to wastewater is limited by its water solubility, which provides a worst-case estimate of the mass concentration that can exist in the wastewater stream slated for treatment in a WWTP. To calculate a water release fraction from the water solubility values, the volume of wastewater produced per unit mass of final product (i.e., m$^3$ wastewater/ tonne produced) needs to be known. Using this information, the water release factor can be calculated using the following formula:

$$Release\ factor\ (\%) = \left( \frac{wastewater\ volume\ \left(\frac{m^3}{tonne}\right) \times water\ solubility\ \left(\frac{mg}{L}\right) \times 1000\ \left(\frac{L}{m^3}\right)}{1.0\times 10^9\ \left(\frac{mg}{tonne}\right)} \right) \times 100 \qquad (2)$$

This allows the water release factors to be calculated for the five water solubility categories. When the water solubility category was described as a numerical range, the geometric mean for the upper and lower limits of the range were used to determine a unique solubility value for that category. For instance, a value of 3.2 mg/L was used to describe the water solubilities ranging from 1 - 10 mg/L.

Several sources of information were used to identify a representative wastewater generation volume normalized for production capacity. These sources are individually highlighted in Table 6 along with the reported and functionally applied wastewater generation volumes.

1. Use in explosives

An early USEPA survey of water usage by explosives manufacturers has yielded a reliable source of information used to determine the wastewater volumes associated with explosives manufacturing. Using the information obtained from site visits, discharge permits, and operating records, the wastewater release from five production sites was found to average 514 gal/ton of product (USEPA, 1975). Using a conversion factors of 0.0038 $m^3$/gal and 0.907 tonne/ton, the wastewater generation for the preparation of explosive formulations at the mixing plants was determined to be 1.8 $m^3$/tonne of product. Although, the plant survey included water use information for large complex facilities that manufactured the chemical intermediates that were then used to manufacture explosives, these values were judged to be unrealistically high given the large volumes of water going into the upstream preparation of precursors. Mixing plants, on the other hand, are smaller facilities located near the explosive use site. These factories are specifically designed for the batch-wise preparation of the final explosive formulation. Considering the aforementioned data, a wastewater generation volume of 2 $m^3$ per tonne of explosive is believed to provide a sufficiently restrictive assessment of the water usage accompanying the manufacturing of explosives (see Table 6).

2. Use in rubber production and processing

The production and processing of synthetic and natural rubbers both rely on the use of solvents for extraction and solvation. A large percentage of these solvents are recovered and reused as an integral part of the production process, but some is released. Unlike synthetic rubber which is polymeric, natural rubber is an elastomer made from the latex found in certain types of vegetation. One type of natural rubber that is being increasingly used in the production of automobile tires uses the sap from the guayule plant as a latex source. A recent life cycle assessment (LCA) reported that 16 kg of solvent are used for latex extraction for every kg of guayule rubber that is produced using a upgraded batch processing method (Azarabadi, et al., 2017). In a separate LCA study, focusing on guayule rubber production by the same method and at the same facility, 68.41 kg of water were reportedly used to produce a kg of natural rubber (Eranki and Landis, 2019). Assuming a solvent density of 1000 kg/$m^3$, the ratio of these two values yields a wastewater generation volume of 4.25 $m^3$/tonne of solvent used. To ensure an adequate safety margin, this value has been rounded upward to 10 $m^3$/tonne (see Table 6), which is the value used to calculate the water release factors for the solvents used in rubber production and processing.

3. Use as blowing agents

Blowing agents encompass a wide array of solid, liquid, and gaseous chemicals including high vapor pressure hydrocarbons such as n-pentane, cyclopentane, and iso-butane (Singh, 2002). Blowing agents function as reactive additives to plastics and polymers that cause the formation of closed cellular structures within the resulting foam product. A life cycle assessment examined the production of an expanded polystyrene resin that utilized n-pentane as the blowing agent during final foam formation (EPS Indusrry Alliance, 2016). A survey of three expanded polystyrene resin manufacturers in Canada, Mexico, and the US yielded information on pentane usage and water consumption. The results showed an average water consumption of 0.829 $m^3$ per 1000 kg of resin and an average pentane usage of 0.0683 tonne per 1000 kg of resin. The quotient for these two numbers yields a wastewater generation volume of 12.1 $m^3$/tonne of blowing agent consumed. Since the production techniques used to manufacture expanded polystyrene resin are highly representative of the processes used to manufacture other foam polymers, the reported waste water generation volume required no further adjustment (see Table 6).

Table 6. Wastewater generation volumes associated each industrial use SpERC

| **Assignments** | **SpERC title** | | |
|---|---|---|---|
| | **explosive use** | **rubber processing** | **blowing agent use** |
| Reported WWTP volume ($m^3$/tonne) | 1.8 | 4.25 | 12.1 |
| Functional WWTP volume ($m^3$/tonne) | 2 | 10 | 12 |
| Source | (USEPA, 1975) | (Azarabadi, et al., 2017, Eranki and Landis, 2019) | (EPS Indusrry Alliance, 2016) |

The functional WWTP were used to calculate the water release factors listed in Table 7 for the three SpERCs highlighted in this guidance document. The values provide a conservative, data-drive, approximation of aqueous solvent release as a function of its water solubility.

As noted above, the water release factors were calculated at the midpoint of the water solubility range. If specific knowledge is available on the water solubility of the solvents being used in a particular application, the release factors may be adjusted to account for the difference between the actual and nominal water solubility values.

Table 7. SpERC water release factors for each water solubility category

| Water solubility (mg/L) | SpERC water release factor (%) | | |
|---|---|---|---|
| | explosive use | rubber processing | blowing agent |
| <1 | 0.0002 | 0.001 | 0.001 |
| 1-10 | 0.0007 | 0.003 | 0.004 |
| 10-100 | 0.007 | 0.03 | 0.04 |
| 100-1000 | 0.07 | 0.3 | 0.4 |
| >1000 | 0.2 | 1.0 | 1.2 |

### *c) Release Factor - soil*

The SpERC-related soil release factors have been compiled from several different sources. As shown in Table 8, a value of zero or 0.01 has been assigned using ECHA-reported default assessments or professional judgement together with available sector knowledge. The soil release factor for the explosive use and rubber processing SpERCs are equivalent to the default values associated with the corresponding ERC (ECHA, 2016).

The soil release values have all been conservatively estimated with the understanding that some release to soil may occur during equipment upsets. These include the spillages that may accompany the transfer or delivery of materials and the development of leaks in pumps, pipes, reactors, and storage tanks. In addition, the supplied soil release factor takes into consideration the wet and dry soil deposition that may accompany the airborne release of a volatile substance. Soil releases from these situations are not expected to be a common occurrence because a majority of the operations covered by these SpERCs take place indoors.

Table 8. SpERC release factors for soil

| Assignments | SpERC title | | |
|---|---|---|---|
| | explosive use | rubber processing | blowing agent |
| ERC | 2 | 4 | 4 |
| Soil release factor (%) | 0.01 | 0.01 | 0 |
| Source | (ECHA, 2016) | (ECHA, 2016) | professional judgement |

### *c) Release Factor – waste*

A thorough and detailed analysis accompanied the assignment of waste release factors for the three SpERCs outlined in this background document. Although a substantial amount of information is available documenting the total amount of different waste types produced annually by solvent users, these data are often in a form that prevents the determination of a normalized release fraction as a function of the production capacity. Life cycle studies can provide useful statistics on waste generation in different industrial use sectors; however, these studies need to be individually examined to determine their relevance to a particular SpERC code.

In this context, waste refers to solvent-containing substances and materials that have no further use and need to be disposed of in a conscientious manner (Inglezakis and Zorpas, 2011). The chemical industry is capable of generating a wide range of hazardous wastes ranging from spent catalysts to a variety of sludges, waste oils, unreacted residues (UNEP, 2014). Waste volumes are dramatically affected by recovery and reuse practices and marketing opportunities that take advantage of any residual value to downstream industries (i.e. industrial symbiosis) (EC, 2015). These practices have allowed the petrochemical industry to conserve resources, optimize operations, and implement new sustainability initiatives that promote alternative applications for these residues and by-products (EEA, 2016).

The waste release factors cited in Table 9 have all been derived from published life cycle assessments (LCAs) that inventory the emissions and wastes generated during the different stages of a product’s service life. These values may be used in the absence of detailed information for a particular industrial operation. These generic values may be supplanted if the actual hazardous waste generation factor is known for the industrial operation under consideration. To guarantee that an adequate margin of protection was built into the determination, an adjustment factor of 10 has occasionally been applied when a reported value was judged to be unrepresentative for the entire range of potential use conditions within a particular industrial sector.

The release factor for explosives was extrapolated from a detailed LCA for the construction and detonation of military grenades (Hägvall, et al., 2004). A portion of this LCA described the waste factors associated with the production of explosive components of the grenade such as ammonium nitrate and trinitrotoluene (TNT). The highest reported waste factor of 0.04% for TNT production provided a good general estimate of the waste generated during the manufacture of explosives of this type. Although the preceding release factor is reasonably indicative of the hazardous waste generation potential in each of the targeted industry sectors, they do not take into consideration the variability associated with using unconventional explosives or use practices. To account for potential differences in the waste generation rates from the various types of explosive, the nominally described value was assumed to represent the lower limit of a range that could vary by as much as 10-fold. To guarantee that an adequate margin of protection was built into the determination, an adjustment factor of 10 has therefore been applied to the explosives SpERC.

The waste fraction associated with the industrial processing of synthetic rubber products has been inferred from an LCA of plastic parts manufacturing using injection moulding machines (Öncel, et al., 2017). The generation of hazardous solvent waste composed of halogenated solvents, washing liquids, and mother liquors was found to range as high as 4.0%. Since the production of synthetic rubber products such as seals and gaskets may involve an extrusion step before vulcanization, the waste factor for plastic parts manufacturing provided reasonably robust surrogate information for the rubber processing SpERC. An LCA for the commercial production of flexible polyurethane foams using an unstated blowing agent provided an estimate of the waste associated with this operation (Plastics Europe, 2005). The amount of incinerated solid waste associated with foam production was determined to be 2.0%. An uncertainty factor was not been applied to the waste factors for rubber processing and blowing agent SpERCs because the cited waste factors include substantial quantities of hazardous waste that has not come into contact with a volatile solvent.

Table 9. SpERC waste release factors and their literature source

| **Assignments** | **SpERC title** | | |
|---|---|---|---|
| | **explosive use** | **rubber processing** | **blowing agent** |
| Release factor (%) | 0.4 | 4.0 | 2.0 |
| Source | (Hägvall, et al., 2004) | (Öncel, et al., 2017) | (Plastics Europe, 2005) |

## 6. Wastewater Scaling Principles

Scaling provides a means for downstream users (DUs) to confirm whether their combination of OCs and RMMs yield use conditions that are in overall agreement with those specified in a SpERC (ECHA, 2014). This consistency check may be accomplished by multiple methods aimed at ensuring that the environmental concentrations resulting from the combination of conditions present at a DU site are less than or equivalent to the levels associated with a SpERC. Scaling principles recognize that a linear relationship exists between the predicted environmental concentration and some, but not all, use determinants (CEFIC, 2010). Factors such as the use amount, the application of emission reduction technologies, wastewater treatment plant capacity, and effluent dilution are all scalable parameters that can be taken into consideration when applying SpERC emission factors to a separate set of circumstances.

The underlying mathematical relation that forms the basis for SpERC scaling is as follows:

$$PEC_{site} = PEC_{SPERC} \times \frac{M_{site}}{M_{SPERC}} \times \frac{RE_{total,site}}{RE_{total,SPERC}} \times \frac{G_{effluent,site}}{G_{effluent,SPERC}} \times \frac{q_{site}}{q_{SPERC}} \times \frac{T_{emission,site}}{T_{emission,SPERC}} \qquad (3)$$

Where:

$PEC_{site}$ – predicted environmental concentration from use at a DU site (g/L)
$PEC_{SPERC}$ – predicted environmental concentration from the use of a SpERC (g/L)

$M_{site}$ – local use amount at a DU site (kg/day)
$M_{SPERC}$ – worst-case estimate of the local use amount associated with a SpERC (kg/day)
$T_{emission,site}$ – number of emission days at a DU site (days)
$T_{emission,SPERC}$ – number of emission days cited for a SpERC (days)
$RE_{total,site}$ – total removal efficiency associated with the application of optional RMMs at a DU site (fraction)
$RE_{total,SPERC}$ – total removal efficiency associated with the application of mandatory RMMs for a SpERC (fraction)
$G_{effluent,site}$ – DU sewage treatment plant flow rate ($m^3$/day)
$G_{effluent,SPERC}$ – SpERC cited sewage treatment plant flow rate ($m^3$/day)
$q_{site}$ – receiving water dilution factor applicable to the DU site (unitless)
$q_{SPERC}$ – receiving water dilution factor applicable to a SpERC (unitless)

Equation 5 shows that a proportionality relationship exists between the use conditions associated with a SPERC and the use conditions that actually exist at a DU site (ECHA, 2008). This relationship forms the basis for ensuring conformity when the wastewater operating conditions differ at a DU site. The scalable parameters described in equation 5 are not equally applicable to every type of environmental risk. As depicted in equations 6-8, the number of scalable parameters increases as the environmental risk of concern become more removed from the wastewater treatment site (CEFIC, 2012). Consequently, the environmental risk to (1) STP microorganisms, (2) organisms residing in the water column and sediment (i.e., freshwater and marine plants and animals), and (3) apical freshwater and marine predators in the aquatic food chain (i.e., secondary poisoning) utilize slightly different scaling equations. Environmental risk is adequately controlled at each trophic level if the following relationships are maintained and the calculations from the SpERC side of the equations are greater than or equal to the results obtained using the site-specific parameters.

Scaling for environmental risk to wastewater treatment plant microorganisms:

$$\frac{M_{SPERC} \times (1-RE_{total,SPERC})}{G_{effluent,SPERC}} \geq \frac{M_{site} \times (1-RE_{total,site})}{G_{effluent,site}} \tag{4}$$

Scaling for environmental risk to freshwater/freshwater sediments, marine water/marine water sediments:

$$\frac{M_{SPERC} \times (1-RE_{total,SPERC})}{G_{effluent,SPERC} \times q_{SPERC}} \geq \frac{M_{site} \times (1-RE_{total,site})}{G_{effluent,site} \times q_{site}} \tag{5}$$

*Scaling for environmental risk to higher members of the food chain (freshwater fish/marine top predator) or indirect exposure to humans by the oral route:*

$$\frac{M_{SPERC} \times T_{emission,SPERC} \times (1-RE_{total,SPERC})}{G_{effluent,SPERC} \times q_{SPERC}} \geq \frac{M_{site} \times T_{emission,site} \times (1-RE_{total,site})}{G_{effluent,site} \times q_{site}} \tag{6}$$

The total removal efficiency ($RE_{total}$) is equal to the product of the removal efficiencies attained using onsite and offsite abatement technologies and is calculated as shown in equation 9.

$$RE_{total,site} = 1 - \left[1 - \left(RE_{onsite,site}\right) \times \left(1 - RE_{offsite,site}\right)\right] \qquad (7)$$

In some cases, an easier and more direct scaling approach may be used that compares individual operational parameters on an item by item basis. This approach allows the individual comparison of local use amounts ($M_{safe}$), emission days per year ($T_{emission,site}$), effluent flow rate ($G_{effluent,site}$), receiving water dilution ($q_{site}$), and total abatement removal efficiency ($RE_{total,site}$). Adequate control of environmental risk exists if $M_{safe} \geq M_{site}$ and the remaining operational conditions comply with the following conditions:

$M_{safe} \geq M_{site}$

$T_{emission,SPERC} \geq T_{emission,site}$

$RE_{total,site} \geq RE_{total,SPERC}$

$G_{effluent,site} \geq G_{effluent,SPERC}$

$q_{site} \geq q_{SPERC}$

$M_{safe}$ (kg/day) is equivalent to the local use amount that yields a risk characterization ratio (RCR) of 1. As such, it represents the maximum tonnage that can be used in conjunction with a prescribed set of operational conditions.

The water release factors provided in this background document represent an additional set of potentially scalable parameters; however, refining the specified values requires detailed justification that goes well beyond the scope of this communication. For this reason, water release factor adjustments are not offered as a feasible alternative when opting for a SPERC-based assessment. DU users need to independently derive and rationalize any release factor modifications that are ultimately used to support their chemical safety assessment.

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