Specific Environmental Release Categories (SpERCs) for the use of solvents and solvent-borne substances in the industrial production and/or use of binders/releasing agents, coatings, cleaners, and metalworking fluids

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 four 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 four factsheets:

1. ESVOC SPERC 4.10a.v3 – Use as binders or release agents
2. ESVOC SPERC 4.3a.v2 – Use in coatings
3. ESVOC SPERC 4.4a.v3 – Use in cleaning agents
4. ESVOC SPERC 4.7a.v3 – Use in metalworking fluids/rolling oils

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 four 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 four 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.

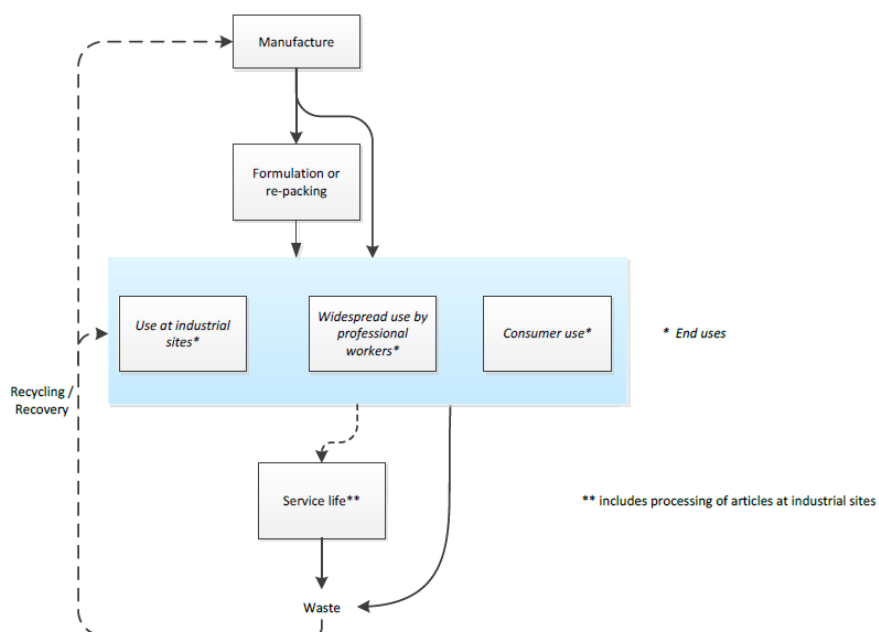Figure 1. ECHA identified life cycle stages and their interrelationship

Table 1. SpERC background information

SpERC Code	Title	Life Cycle Stage (LCS)	Sector of Use (SU)	Chemical Products Category (PC)	Use Description
ESVOC SPERC 4.10a.v3	Use as binders or release agents	Industrial end-use	SU0 other	PC24 lubricants, greases, release products	Covers the use as binders and release agents including material transfers, mixing, application (including spraying and brushing), mould forming and casting, and handling of waste.
ESVOC SPERC 4.3a.v2	Use in coatings	Industrial end-use	SU0 other	PC9a coatings and paints, thinners, paint removers	Covers the use in coatings (paints, inks, adhesives, etc.) including exposures during use (including materials receipt, storage, preparation and transfer from bulk and semi-bulk, application by spray, roller, spreader, dip, flow, fluidized bed on production lines and film formation) and equipment cleaning, maintenance and associated laboratory activities.
ESVOC SPERC 4.4a.v3	Use in cleaning agents	Industrial end-use	SU9 other	PC35 washing and cleaning products	Covers the use as a component of cleaning products including transfer from storage, pouring/unloading from drums or containers. Exposures during mixing/diluting in the preparatory phase and cleaning activities (including spraying, brushing, dipping, wiping, automated and by hand), related equipment cleaning and maintenance.
ESVOC SPERC 4.7a.v3	Use in metal working fluids/rolling oils	Industrial end-use	SU9 other	PC25 metal working fluids	Covers the use in formulated MWFs/rolling oils including transfer operations, rolling and annealing activities, cutting/machining activities, automated and manual application of corrosion protections (including brushing, dipping and spraying), equipment maintenance, draining and disposal of waste oils.

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.

3.1. Conditions of use

All four 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 4.10a.v3	ESVOC SPERC 4.3a.v2	ESVOC SPERC 4.4a.v3	ESVOC SPERC 4.7a.v3
wet scrubbers	50 - 99	70	Z	X	X	Z
thermal oxidation	95 - 99.9	95	X	X	X	X
solid adsorbent	80 - 95	80	X	X	X	X
membrane separation	<99	80	Z	Z	Z	Z
biofiltration	75 - 95	75	Z	Z	Z	Z
cold oxidation	80 - >99.9	80	Z	Z	Z	Z
air filtration	70 - 99	70	Z	X	Z	X

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 macro-porous 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 four SpERCs identified in this guidance document have 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 four SpERCs.

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

Tonnage	SpERC title			
	ESVOC SPERC 4.10a.v3	ESVOC SPERC 4.3a.v2	ESVOC SPERC 4.4a.v3	ESVOC SPERC 4.7a.v3
Local use rate (kg/day)	25,000	50,000	5,000	25,000
Emission days	100	300	20	20
Fractional local EU tonnage	100%	100%	100%	100%
Fractional regional EU tonnage	100%	100%	100%	100%
Rationale	tanker truck shipments	tanker truck shipments	tanker truck shipments	published citation

The estimated local use rate at sites manufacturing binders/release agents, coatings, and cleaning agents were 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 1 per day for the use in the production of binders/release agents, 1 per week (assuming a 5-day work week) for the formulation of cleaning agents, and 2 per day for use in coating preparations. The equation used to calculate these use rates is as follows:

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

The use rate associated with the preparation of metalworking fluids and rolling oils considered published accounts of the site tonnage at plants manufacturing lubricants in the United Kingdom (OECD, 2004). Facilities manufacturing specialty products such as metalworking fluids are often small operations that prepare a range of lubricants, greases, and oils. The production capacity for these small independent operations can range from 500 - 10,000 tonnes/day. Since this use rate represents includes the production for all types of lubricants, the value at the lower end of this range was judged to be more representative of the production volume for metalworking fluids alone. The value of 500 tonnes/year is equivalent to 25,000 kg/day for a site operating 20 days/year. The equation used to calculate the formulation use rate is as follows:

$$Use\ rate\ \left(\frac{kg}{day}\right) = \frac{plant\ capacity\ \left(\frac{tonnes}{year}\right) \times 1000\ \left(\frac{kg}{tonne}\right)}{operating\ period\ \left(\frac{days}{year}\right)} \quad (2)$$

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 for each of the SpERCs described in this guidance document vary as shown in 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; whereas the value of 100 days is applicable to operations where the use amounts are greater than 1,000 tonnes/year and less than 5,000 tonnes/year. A value of 20 days/year is applied when the industrial use if less than 1,000 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 four SpERCs considered herein.

Table 5. SpERC release factors for air

Assignments	SpERC title			
	release agent use	coating use	cleaner use	metalworking fluid use
Air release factor (%)	98	98	98	5
Source	(ECHA, 2016)	(OECD, 2009)	(ECHA, 2016)	(OECD, 2004)

1. Use in releasing agents and binders

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 a non-reactive processing aid at industrial site (no inclusion into or onto article). Processing aids include the use of solvents in cleaners, paints, adhesives and other products. 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).

2. Use in coatings

Air emission estimates for the industrial application of solvent-borne coatings have been previously determined in an authoritative review that examined the loss of volatiles following the use of alternative coating processes (OECD, 2009). An air release factor of 98% was estimated to occur when a coating was applied to furniture using a flatline finishing process that involves the use of brush rollers or a liquid curtain for the transfer. This value was selected for use in the coating SpERC since it provides a more judicious and practical estimate than the value of 94% for the spray application of a coating to furniture.

3. Use in cleaning 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 aid at industrial site (no inclusion into or onto article). Processing aids include the use of solvents in cleaners, paints, adhesives and other products. 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).

4. Use in metalworking fluids

An emission scenario document for lubricants provided the basis for establishing a metalworking fluid air release factor (OECD, 2004). Misting and evaporative losses from the use of conventional soluble oils containing a wide array of potentially volatile additives, corrosion inhibitors, emulsifiers, and coupling agents was reported to be 5%. This factor provides a verifiable and well substantiated estimate of the air release that accompanies the milling and machining of metal parts using a metal working fluid that is automatically or manually processed to remove the metal filings (i.e., swarf).

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:

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

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:

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

This allows the water release factors to be calculated for 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. In some cases, a reasonable and definitive information database could not be located in the scientific literature. The absence of information was offset using expert professional judgement and industry sector knowledge acquired by a variety of means including networking opportunities, trade association meetings, and social media interactions. Sector knowledge was vital in establishing the wastewater generation volumes associated with the use of solvents in the industrial manufacture or use of releasing agents and cleaning agents.

1. Use in releasing agents and binders

Aluminum die casting is a commonly used method to manufacture automobile parts in the European Union. The process involves the pressurized injection of molten aluminum or other metal into a die or mold that is allowed to cool before the part is separated. The metal part then moves to a finishing area where trimming, machining, and cleaning takes place. To facilitate the release of the part, a die release lubricant mixed with water is sprayed onto each half of the die after each part production cycle. Before lubricant application, cooling water is used to lower the die temperature, which allows the lubricant to adhere to the die. This wash step and the aqueous dilution of the release lubricant before spray application are the primary determinants of the overall wastewater generation volume from this step in the process.

Metal die casting is known to be a very water intensive operation, with large volumes used for both lubricating the mold and for cooling. The stock lubricants used as release agents are often diluted with water prior to mold application. The aqueous dilution ratio may range from 30:1 (v/v) up to 200:1 (v/v) depending on the metal casting process and the part being manufactured (Natesh, 2014). A dilution ratio of 50:1 is commonly observed in many die casting operations (NADCA, 2015). Following application, the used releasing agent is disposed of in the wastewater stream and is not recycled to any appreciable degree. As such, the volume of water use can be directly related to the dilution factor. A 50:1 dilution would be equivalent to a water usage volume of 50 m^3 per tonne of lubricant assuming a stock lubricant density of 1000 kg/m^3. This value is both prudent and practical since it does not overly compensate for those processes where a releasing or binding agent requires far less water use or a greater volume of lubricant.

2. Use in coatings

Wastewater generation for the coating SpERCs was assessed using batch data from an industry manufacturing 20 tons/day of a water-based paint (Kutluay, et al., 2004). Wastewater generation from the cleaning of mixing tanks, filters, holding tanks, and filling equipment totalled 4.6 m^3/day or 0.23 m^3 per tonne of paint. These values provide a representative example of the water usage that would be expected in other segments of the coating industry. Likewise, since the wastewater volume was associated with the production of water-based coatings in a batch-wise manner, the measurement is expected to be more conservative than other more automated operations formulating products that are not water soluble. To account for any uncertainties in the reporting and to ensure an adequate margin of environmental protection, the reported wastewater generation rate of 0.23 m^3/tonne was increased to 20 m^3/tonne. This modification helps guarantee that the wastewater generation from other types of high-volume coating manufacturing operations taken into appropriate consideration.

3. Use in cleaners

Industrial cleaning agents include a wide variety of products capable of removing grease, grime, and oily residues from a solid surface. A worse-case determination of wastewater generation volumes associated with industrial cleaning operations focused on the removal of residual flux from printed circuit boards (Duchi and Laügt, 2014).   This process uses cleaning agents such as detergents, petroleum distillates, formulated hydrocarbons, glycols, or modified alcohols to remove contaminants such as fingerprints, solder rosins, and residual fluxes from the circuit boards. A cost analysis of alternative methods for cleaning printed circuit boards suggests that wastewater generation is greatest when an aqueous based cleaning agent is employed (Savidakis, et al., 2010).   The evaluation found cleaner losses of 5.5 gallons per hour (0.21 m^3/hr) due to the drag-out that occurs when the boards are remove from the wash bath. The corresponding water usage for this cleaning scenario was 300 gallons per hour, which is equivalent to 1.13 tonnes/hr assuming a density is 1000 kg/m^3. The ratio of the two usage rates yields a wastewater generation volume of 0.02 m^3/tonne using a conversion factor of 0.0038 m^3/gallon.

Since the wastewater generation volume associated with the circuit board cleaning may not be entirely representative of the numerous industrial processes that employ a solvent-based cleaning agent, the application of an adjustment factor seems appropriate. Use of an adjust factor ensures that the value provides a worst-case determination of wastewater generation and compensates for other industrial operations where the water usage may be greater. When an adjustment of 5 is applied to the wastewater volume of 0.02 m^3/tonne, a final value of 0.1 m^3/tonne is obtained.

4. Use in metal working fluids

Wastewater generation for the metalworking fluid SpERCs was assessed using published information from the scientific or technical literature. The aqueous discharge associated with the blending of a metalworking fluid was assessed for a UK site producing 10,000 tonnes of lubricant per year (OECD, 2004). The wastewater discharge volume for this site was stated to be 100 L/tonne (0.1 m^3/tonne). Since the volume of wastewater is highly dependent on the housekeeping and maintenance frequency, the preceding value may not be entirely representative of the conditions at other facilities where metalworking fluids are manufactured or utilized. Consequently, an adjustment factor of 10 was applied to obtain a functional wastewater generation volume of 1.0 m^3/tonne for the metalworking fluid SpERC.

Table 6. Wastewater generation volumes associated each industrial use SpERC

Assignments	SpERC title			
	release agent use	coating use	cleaner use	metalworking fluid use
Reported WWTP volume (m³/tonne)	50	0.23	0.02	0.1
Functional WWTP volume (m³/tonne)	50	20	0.1	1.0
Source	(NADCA, 2015)	(Kutluay, et al., 2004)	(Savidakis, et al., 2010)	(OECD, 2004)

Using these data, the water release factors listed in Table 7 were calculated for the four SpERCs highlighted in this guidance document. The values provide a conservative worst-case 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 (%)			
	release agent use	coating use	cleaner use	metalworking fluid use
<1	0.005	0.002	0.00001	0.0001
1-10	0.017	0.007	0.00003	0.0003
10-100	0.17	0.07	0.0003	0.003
100-1000	1.67	0.7	0.003	0.03
>1000	5	2.0	0.01	0.1

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, professional judgement and available sector knowledge, or published OECD emission scenario information. An evaluation of soil releases during coating manufacturing showed that there would be no direct releases to soil under normal operating conditions (OECD, 2009). Likewise, an examination

of the environmental releases of metalworking and cutting fluids failed to show a measurable release of these products to soil during the blending process (OECD, 2004).

Table 8. SpERC release factors for soil

Assignments	SpERC title			
	release agent use	coating use	cleaner use	metalworking fluid use
ERC	4	4	4	4
Soil release factor (%)	0	0	0	0
Source	professional judgement	(OECD, 2009)	professional judgement	(OECD, 2004)

The soil release values have all been conservatively estimated with the understanding that very small releases 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. The soil affected by minor spills is often promptly attended to and the area cleaned to ensure that there is no residual release. Since a majority of the operations covered by these SpERCs take place indoors, soil spills are not expected to be a common occurrence.

c) Release Factor – waste

A thorough and detailed analysis accompanied the assignment of waste release factors for the four 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).

Three of the four waste release factors cited in Table 9 have 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.

An LCA for the manufacture of base fluids used in the blending of lubricants provided a relevant foundation for determining waste factors for the releasing agents and metalworking fluids SpERCs (Våg, et al., 2002). The esterification process leading to the production of lubricant base fluids from rapeseed oil and petroleum-based polyols resulted in a waste factor of 1.0%. This value was judged to be representative of the hazardous waste generation potential associated with the manufacture and/or use of binders, releasing agents, metalworking fluids, and cutting oils.

Unlike the preceding SpERCs, the waste release factor for the use of solvents in the preparation of coating formulations was taken from an ESD (OECD, 2009). A waste release factor of 0.5% was calculated to be indicative of the residues generated during the batch production of an organic solvent-borne coating. Although the preceding release factors are 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 manufacturing or use practices. The use of a volatile degreasing agent in the metal working industry provided a reasonable estimate of the waste associated with the industrial use of cleaning products (Vollebregt and Terwoert, 1998). The production and use of a mixture of dearomatized C10-C12 hydrocarbons to degrease and treat metal parts was associated with production of 0.4% of solid waste.

Table 9. SpERC waste release factors and their literature source

Assignments	SpERC title			
	release agent use	coating use	cleaner use	metalworking fluid use
Release factor (%)	10.0	5.0	4.0	10.0
Source	(Våg, et al., 2002)	(OECD, 2009)	(Vollebregt and Terwoert, 1998)	(Våg, et al., 2002)

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:

$$PEC_{site} = PEC_{SPERC} \times \frac{M_{site}}{M_{SPERC}} \times \frac{RE_{total,site}}{RE_{total,SPERC}} \times \frac{G_{effluent,site}}{G_{effluent,SPERC}} \times \frac{q_{site}}{q_{SPERC}} \times \frac{T_{emission,site}}{T_{emission,SPERC}} \qquad (5)$$

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 (m³/day)

$G_{effluent,SPERC}$ – SpERC cited sewage treatment plant flow rate (m³/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:

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

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

$$\frac{M_{SPERC} \times (1 - RE_{total,SPERC})}{G_{effluent,SPERC} \times q_{SPERC}} \geq \frac{M_{site} \times (1 - RE_{total,site})}{G_{effluent,site} \times q_{site}} \tag{7}$$

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:

$$\frac{M_{SPERC} \times T_{emission,SPERC} \times (1 - RE_{total,SPERC})}{G_{effluent,SPERC} \times q_{SPERC}} \geq \frac{M_{site} \times T_{emission,site} \times (1 - RE_{total,site})}{G_{effluent,site} \times q_{site}} \tag{8}$$

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.

$$RE_{total,site} = 1 - \left[1 - \left(RE_{onsite,site} \right) \times \left(1 - RE_{offsite,site} \right) \right] \tag{9}$$

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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