Specific Environmental Release Categories (SpERCs) for the use of solvents and solvent-borne substances in the industrial production and/or use of water treatment chemicals, polymers, mining chemicals, and fuels

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 3.22a.v3 – Use in water treatment
2. ESVOC SPERC 4.21a.v2 – Use in polymer processing
3. ESVOC SPERC 4.23.v2 – Use in mining operations
4. ESVOC SPERC 7.12a.v3 – Use as a fuel

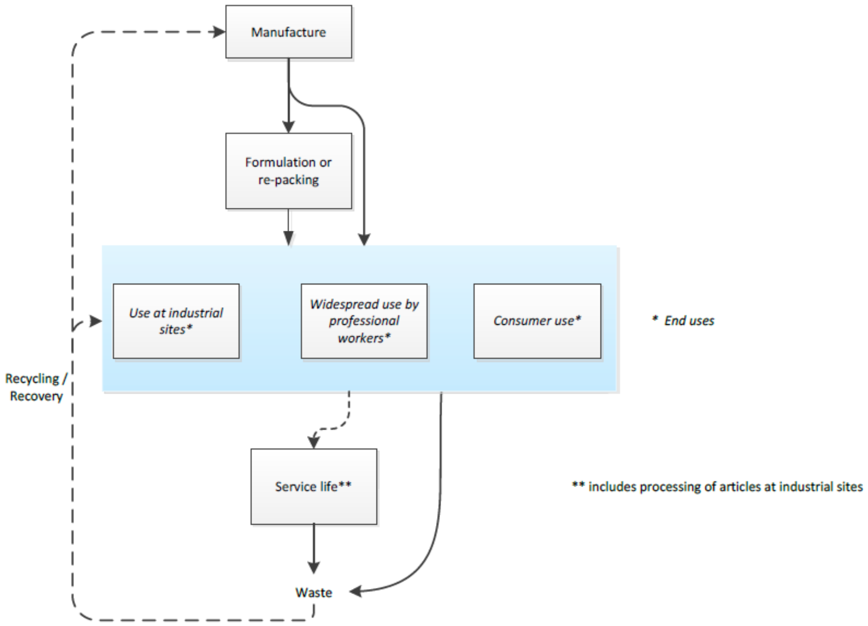
Since these newly released SpERC factsheets include some corrections and or modifications, the version number has been changed to reflect the updates.

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



* *End uses*

** includes processing of articles at industrial sites

Table 1. SpERC background information

SpERC Code	Title	Life Cycle Stage (LCS)	Sector of Use (SU)	Chemical Products Category (PC)	Use Description
ESVOC SPERC 3.22a.v3	Use in water treatment	Industrial end-use	SU0 other	PC20 processing aids such as pH-regulators, flocculants, precipitants, neutralizing agents	Covers the use of the substance for the treatment of water at industrial facilities in open and closed systems.
ESVOC SPERC 4.21a.v2	Use in polymer processing	Industrial end-use	SU12 manufacture of plastic products, including compounding and conversion	PC32 polymer preparations and compounds	Processing of formulated polymers including material transfers, additives handling (e.g. pigments, stabilisers, and fillers, plasticisers), moulding, curing and forming activities, material re-works, storage and associated maintenance.
ESVOC SPERC 4.23.v2	Use in mining operations	Industrial end-use	SU2a mining (without offshore industries)	PC40 extraction agents	Covers the use of the substance in extraction processes at mining operations, including material transfers, winning and separation activities, and substance recovery and disposal.
ESVOC SPERC 7.12a.v3	Use as a fuel	Industrial end-use	SU8 manufacture of bulk, large scale chemicals (including petroleum products)	PC13 fuels	Covers the use as a fuel (or fuel additive) and includes activities associated with its transfer, use, and equipment maintenance.

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 and/or outdoor 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 3.22a.v3	ESVOC SPERC 4.21a.v2	ESVOC SPERC 4.23.v2	ESVOC SPERC 7.12a.v3
wet scrubbers	50 - 99	70	X	Z	X	Z
thermal oxidation	95 - 99.9	95	X	X	X	X
solid adsorbent	80 - 95	80	Z	X	Z	Z
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	Z	Z	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 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, biotrickle filtration, and bioscrubbing. 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).

4.2. 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 3.22a.v3	**ESVOC SPERC 4.21a.v2**	**ESVOC SPERC 4.23.v2**	**ESVOC SPERC 7.12a.v3**
Local use rate (kg/day)	100	50,000	10,000	5,000,000
Emission days	300	300	20	300
Fractional local EU tonnage	100%	100%	100%	100%
Fractional regional EU tonnage	100%	100%	100%	100%
Rationale	published citation	tanker truck shipments	tanker truck shipments	published citation

The estimated local use rate at sites processing polymers or using mining chemicals was based on professional judgement and takes 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 polymer processing and 2 per week (assuming a 5-day work week) for the use of mining chemicals. 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 water treatment chemicals was surmised from the use concentration of polyacrylamide as a coagulant for the treatment of wastewater and an examination of the capacity of typical industrial WWTPs used by the paper industry. The stated maximum use concentration of polyacrylamide for influent and effluent treatment has been reported to be 10 mg/L (0.01 kg/m^3) (OECD, 2004). A survey of the capacity for the industrial wastewater treatment at paper manufacturing facilities found that the influent flowrate was often less than 10,000 m^3/day (Niu, et al., 2016). The product of these two variables yields a local use rate of 100 kg/day, which was judged to provide a reasonably representative approximation of water treatment chemical usage under various conditions.

The use rate of fuels was derived from the reported consumption of jet fuel by airports in the U.S. (NREL, 2014). A survey of the yearly jet fuel usage at small to medium sized airports in various regions of the U.S. found that the rate did not exceed 600 million gallons per year, which is equivalent to 5,230,386 kg/day when the density of jet fuel (840 kg/m3) is taken into consideration. This information indicated that a daily fuel usage value of 5,000,000 kg/day provided a reliable approximation that was sufficiently inclusive of other industrial fuel use scenarios. The equation used to calculate the fuel use rate is as follows:

$$Use\ rate\ \left(\frac{kg}{day}\right) = \frac{jet\ fuel\ consumed\ \left(\frac{gals}{year}\right) \times fuel\ density\ \left(\frac{kg}{m^3}\right)}{365\ \left(\frac{days}{year}\right) \times 264\ \left(\frac{gal}{m^3}\right)} \qquad (2)$$

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 varies 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; whereas the value of 20 days/year is applied when the industrial use if less than 1,000 tonnes/year (ECHA, 2016). Consequently, the more characteristic value of 300 days/year was applied. The tonnage cut-off limits cited above represent the maximum use amount at a single site. The default value of 20 days/year was not used for the water treatment chemical SpERC, since available sector knowledge revealed that these substances are used on a nearly daily basis.

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 may 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 with several water solubility categories to define any relevant 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 for several of the SpERCs described in this background document. When reliable information was unavailable for the solvents used in a particular industrial application, a worst-case default estimate was applied that relied heavily on expert judgement and sector knowledge. Otherwise, published air release factors were applied once the information was suitably vetted and analyzed.

1. Use as a water treatment chemical

Water treatment chemicals include a large number of products available for use in various industrial applications. These products include algaecides, antifoams, biocides, defoamers, coagulants, corrosion inhibitors, flocculants, neutralizing agents, oxygen scavenges, pH conditioners, scale inhibitors, and a variety of the other agents. The vast majority of chemicals in these categories are either inorganic salts or high molecular weight polymers. The substances are characterized by their low vapor pressure which limits the likelihood of an air emission during their use. As such, a search was performed to identify a water treatment with chemico-physical properties that were representative of the entire chemical class. The flocculant, N-(n-octyl)-2-pyrrolidinone (NOP, CAS# 2687-94-7) typified this class of chemicals and its environmental distribution was examined using SimpleTreat 4.0, a multi-media box model capable of describing the fate of a chemical in a sewage treatment plant (Maltesh, et al., 2002, RIVM, 2015). The model was populated with chemico-physical properties extracted from ECHAs registration summary for this substance (ECHA, 2019). These included a water solubility of 1140 mg/L, a vapor pressure of 0.08 Pa, and an octanol-water partition coefficient (Kow) of 14,125 at 20 °C.

SimpleTreat was operated as a 6-box model that included aerobic biological treatment and solid/liquid separation without the removal of any solids in a primary clarifier. These conditions are more representative of an industrial wastewater treatment plant where the flocculant is added to a mixing tank located upstream of the activated sludge unit. NOP was assumed to be loaded into the waste stream at the maximum rate of 100 kg/day. The total wastewater flow through the treatment plant was set at the default value of 200 m3/day. Distribution of the flocculant to air, water and suspended solids was assessed by setting the biodegradation rate constant to 0 hr^{-1}, which provided a worst-case estimate of the emission factors. The simulation showed that 0.03% of the NOP was released to air, 82% to water, and 18% bound to sludge.

2. Use in polymer processing and as a mining chemical

For two of the SpERCs, polymer processing and use in the mining industry, suitably categorized air emission factors were obtainable from the A-Tables published by the European Commission and listed in Appendix 1 of the Technical Guidance Document (TGD) on Risk Assessment Part II (EC, 2003). Use of these A-Tables requires the proper identification of the use characteristics associated with a particular industrial application. These identifiers are presented in Table 5 for the polymer processing and mining SpERCs.

Table 5. Information used to compile the list of air release factors

Identifiers	**SpERC title**	
	polymer processing	**mining chemical use**
Industry category	IC=11 Polymers industry	IC=8 Metal extraction, refining and processing industry
Main category	**NA**	III Non-dispersive industrial use or processing of intermediates
Use category	48 (solvents)	NA
A-table number	A3.11	A3.7

NA – not applicable

4. Use as a fuel

The industrial use of liquid fuels occurs in a wide variety of operations where there is a demand for heat, horsepower, or electricity. Given the wide range in volatility for the various hydrocarbon fuels, separate air emission factors were identified for fuels with vapour pressures less than or greater than 1000 Pa. For fuels with a vapor pressure greater than 1000 Pa, the ERC 7 default value of 5% was as an air release factor (ECHA, 2016). The listed default value has been attributed to the use of a functional fluid at an industrial site, but does not take into consideration the impact of vapor pressure on the magnitude of atmospheric release. Since the volatility of many fuels is substantially less than middle distillate fuels such as kerosene, a separate vapor pressure category was created for fuels with a volatility less than 1000 Pa.

Many generators use fossil fuels such as fuel oil and diesel to generate the electrical power used to manufacture a wide range of products. An investigation of the hydrocarbon air emissions associated with the use of diesel-powered generators in Nigeria included measurements of fuel consumption

(Okedere, et al., 2015). The average consumption of diesel fuel by 12 generators powering a variety of spinning, weaving, printing or dying operations was 0.0081 L/sec. whereas the average hydrocarbon emission factor was 0.0385 g/sec. After correcting for the density of diesel fuel (0.832 kg/L), the ratio of these two values yields an average air emission factor of 0.57%. This value has rounded upward to 0.6% for fuels with a vapor pressure less than 1000 Pa, which includes diesel fuel (VP = 500-<5000 Pa @ 37.8 °C/100 °F) (CONCAWE, 2010).

Table 6 provides a listing of the emission factors and their associated literature sources for the two SpERCs examined. As shown in the Table, the air release factor for the mining chemical SpERC is unaffected by the vapour pressure of the solvent being used and has been set at a constant value of 25%. In contrast, the release factor for the polymer processing SpERC varies across four vapour pressure categories.

Table 6. SpERC release factors for air

Vapour pressure (Pa)	**SpERC air release factor (%)**			
	water treatment	**polymer processing**	**mining chemical use**	**fuel use**
>10000	See text	75	25	See text
1000-10000		50	25	
100-1000		25	25	
<100		10	25	

The air emission factors shown in Table 6 and cited in the text above 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

Several sources of information were used to identify a representative water release factor. These sources are individually highlighted in Table 7 along with the assigned value. The values provide a conservative worst-case approximation of aqueous solvent release regardless of water solubility. In some cases, a reasonable and definitive information database could not be located in the scientific literature. The absence of information was counterbalanced using expert professional judgement and industry sector knowledge acquired by a variety of means including networking opportunities, trade association meetings, and social media interactions.

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.

1. Use as a water treatment chemical

The water release factor for water treatment chemicals was determined using the SimpleTreat model to map the releases of a flocculant added to a wastewater stream. Details regarding the modeling assumptions, chemical properties, and treatment plant operation are described above for the release factors to air. A release factor of 82% was estimated for the flocculant, N-(n-octyl)-2-pyrrolidinone, which aids particle aggregation and removal from a wastewater stream. The environmental distribution of this chemical was examined when SimpleTreat was operated as 6-box model without any biodegradation of the added flocculant (RIVM, 2015).

2. Use in polymer processing and as a mining chemical

Wastewater generation for the polymer processing and mining chemical SpERCs was assessed using published information supplied in the A-Tables listed in Appendix 1 of the Technical Guidance Document (TGD) on Risk Assessment (Part II). These values represent a worst-case estimate that was derived by experts and informed authorities from the European Commission, Member States, and public interest groups.

3. Use as a fuel

A water release factor for industrial fuel use was derived from a life cycle assessment of heavy fuel oil use in a German power plant (IEA, 2017). The study found that 0.037 mg of unspecified hydrocarbons and 0.057 mg of unspecified oils were released to wastewater for every megajoule (MJ) of fuel oil consumed. The total release of 0.094 mg/MJ is equivalent to a water release fraction of 0.0004% after adjusting for the net calorific value of fuel oil which is 40.9 MJ/kg (Staffell, 2011). To account for the use of fuels with a higher water solubility, this value was adjusted upward by 2.5-fold to obtain an overall water emission factor of 0.001%.

Table 7. SpERC release factors for water

Assignments	**SpERC title**			
	water treatment	**polymer processing**	**mining chemicals**	**fuel use**
Water release factor (%)	82	0	50	0.001
Source	(RIVM, 2015)	(EC, 2003)	(EC, 2003)	(IEA, 2017)

c) Release Factor - soil

The SpERC-related soil release factors have been compiled from several different sources. As shown in Table 8, values have been assigned using either expert judgement or the information supplied in the A-Tables published in Appendix 1 of the Technical Guidance Document (TGD) on Risk Assessment (Part II) (EC, 2003). The soil release fraction for the polymer processing and mining chemical SpERCs were taken directly from the A-Tables; whereas professional judgement and available sector knowledge were crucial to the assignment of soil release factors for the SpERCs covering the use of water treatment chemicals and hydrocarbon fuels. For the two latter SpERCs, the release to soil was considered to be inconsequential given the requisite use conditions or prohibitive in accordance with recognized regulatory requirements.

The soil release values have all been conservatively estimated with the understanding that small soil releases 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 supplied soil release factor take into consideration these factors as well as the wet and dry soil deposition that may accompany the airborne release of a volatile substance.

Table 8. SpERC release factors for soil

Assignments	**SpERC title**			
	water treatment	**polymer processing**	**mining chemical use**	**fuel use**
ERC	3	4	4	7
Soil release factor (%)	0	0.001	5.0	0
Source	professional judgement	(EC, 2003)	(EC, 2003)	professional judgement

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 product formulators and users 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 waste factor associated with the use of paper chemicals was taken from an LCA describing the production of office paper from recycled supplies (DEFRA, 2012). The LCA focused on the reprocessing of closed-loop recycled paper sent back to the paper mill by businesses operating in Europe. The pulp generated from this recycled paper is initially treated with a variety of chemicals to aid in the toner removal and promote slurry formation. The operation resulted in the generation of 1.13 kg/tonne (0.013%) of unrecovered industrial waste that could contain residual amounts of paper-making chemicals. This factor was adopted without modification or the application of an uncertainty factor since the facility provides a representative example of the practices employed by other facilities using water treatment chemicals.

An LCA for polymer manufacturing provided a solid foundation for determining an appropriate waste factor for the polymer processing SpERC (Plastics, 2005). The assessment examined the production of high-density polyethylene from olefin monomers. The amount of incinerated solid waste generated during polymer production was stated to 870 mg/kg (0.09%). This value was rounded upward to 0.1% to ensure an adequate depiction of this life cycle stage. An uncertainty factor of has not been applied to this value because the quantity of hazardous waste is not expected to appreciably vary for other polymer processing operations.

The waste associated with the use of chemicals in mining industry has been documented for a copper mining and smelting operation (ICA, 2013). An LCA covering all phases of copper cathode production from mining through refining yielded a robust assessment of the wastes produced by this industry. The amount of hazardous waste resulting from the various processing stages, including leaching and solvent extraction, was found to be 0.003 kg/tonne (0.0003%). The waste factor is representative copper refining operations at mining sites on four continents. An uncertainty factor of 10 has been applied to this value based on the anticipated variations for different types of mining operations. The application of this adjustment factor resulted in a final waste release factor of 003%.

The waste factor for the SpERC covering industrial fuel use was adapted from an examination of gasoline production and use in passenger cars (Morales, et al., 2015). The evaluation revealed that 2.1 ml of hazardous waste was incinerated per km driven. At the stated fuel mileage of 150 ml/km, a waste release factor of 1.4% was derived. To ensure broad representation across a range of use conditions, this value which was rounded upward to 2%. An uncertainty factor has not been applied to this value since the waste associated with industrial fuel use is expected to less than the value obtained for this sweeping and all-inclusive analysis.

Table 9. SpERC waste release factors and their literature source

Assignments	**SpERC title**			
	water treatment	**polymer processing**	**mining chemicals**	**fuel use**
Release factor (%)	0.1	0.1	0.003	2.0
Source	(DEFRA, 2012)	(Plastics, 2005)	(ICA, 2013)	(Morales, et al., 2015)

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:

$$PEC_{site} = PEC_{SPERC} \times \frac{M_{site}}{M_{SPERC}} \times \frac{RE_{total,site}}{RE_{total,SPERC}} \times \frac{G_{effluent,site}}{G_{effluent,SPERC}} \times \frac{q_{site}}{q_{SPERC}} \times \frac{T_{emission,site}}{T_{emission,SPERC}} \quad (4)$$

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 4 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 4 are not equally applicable to every type of environmental risk. As depicted in equations 5-7, 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:

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

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

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

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:

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

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 8.

$$RE_{total,site} = 1 - [1 - (RE_{onsite,site}) \times (1 - RE_{offsite,site})] \qquad (8)$$

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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