
Specific Environmental Release Categories (SpERCs) for the industrial manufacture, formulation, and intermediate use of solvents and solvent borne substances

Introduction

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

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

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

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



1. Title

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

1. ESVOC SPERC 1.1.v2 – Manufacture of a substance
2. ESVOC SPERC 2.2.v2 – Formulation & (re)packing of substances and mixtures
3. ESVOC SPERC 6.1a.v2 – Use as an intermediate

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 three SpERCs highlighted in this guidance document cover several different life cycle stages including manufacture, formulation/re-packing and industrial end-use. The interrelationship between these stages as envisioned under REACH is depicted in Figure 1 (ECHA, 2015). Individual SpERCs have been created for the manufacturing, formulation/repacking, and industrial end-use stages. Use descriptors have been assigned in accordance with the naming conventions outlined by ECHA. The expressions and descriptions used to characterize the three SpERCs in Table 1 are consistent with the list of standard phrases that accompanied the creation of Generic Exposure Scenarios (GESs) to describe the industrial production and use of solvents (ESIG/ESVOC, 2017). The use of standard phrases in these SpERC descriptions provides consistency and harmonization when used by manufacturers/importers and downstream users to create their exposure scenarios.

Figure 1. ECHA identified life cycle stages and their interrelationship

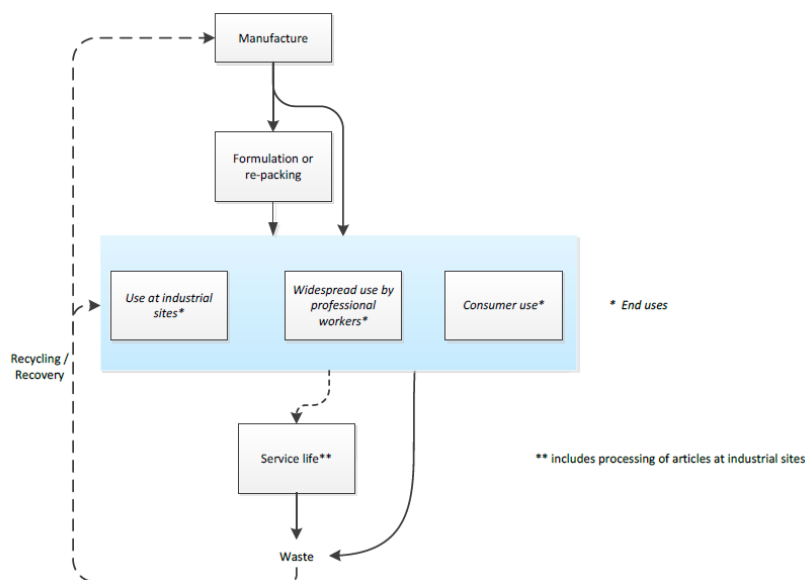


Table 1. SpERC background information

SpERC Code	Title	Life Cycle Stage	Description	Reference
ESVOC SPERC 1.1.v2	Manufacture of substance (industrial): solvent-borne	manufacture	Includes the commercial production of solvents and other large volume volatile organic chemicals from basic raw material feedstocks. Activities include recycling/recovery, material transfer, storage, maintenance, loading (including marine vessel/barge, road/rail car and bulk container), sampling, and associated laboratory activities.	(Money, et al., 2011)
ESVOC SPERC 2.2.v2	Formulation & (re)packing of substances and mixtures (industrial): solvent-borne	formulation	Covers the formulation, packing and re-packing of the substance and its mixtures in batch or continuous operations, including storage, materials transfers, mixing, tableting, compression, pelletisation, extrusion, large- and small-scale packing, sampling, maintenance and associated laboratory activities.	(Money, et al., 2011)
ESVOC SPERC 6.1a.v2	Use as an intermediate	industrial end-use	Use of the substance as an intermediate (not related to Strictly Controlled Conditions). Includes recycling/recovery, material transfers, storage, sampling, associated laboratory activities, maintenance and loading (including marine vessel/barge, road/rail car and bulk container).	(ESIG/ESVOC, 2017)

3. Operational conditions

The operating conditions for a particular production process, formulation operation, or downstream 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 three SpERCs are applicable to indoor chemical facilities that operate using any of several types of closed-continuous reactors that minimize releases to the environment (Walas, 1997). Examples include continuous stirred tank, fluidized bed, and tubular reactors. In most cases, these processes do not use water as an extraction solvent, an adsorbent, or a reaction medium (OECD, 2011). The primary source of treatable wastewater from these processes results when drums, tanks, and transfer equipment are cleaned.

Biological wastewater treatment (WWT) may involve the use of both industrial and municipal WWT facilities. The prevalence of each type of facility was assessed in 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. Despite the limited reliance on municipal treatment facilities, their usage is conservatively assumed to exist as a normal operating condition during the production, formulation, and downstream use of solvents.

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, any residual waste generated during the production and industrial use of a volatile solvent needs to be 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, 2017b).

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 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

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 1.1.v2 manufacture	ESVOC SPERC 2.2.v2 formulation	ESVOC SPERC 6.1a.v2 intermediate use
wet scrubbers	50 - 99	70	Z	X	X
thermal oxidation	95 - 99.9	95	Z	X	Z
solid adsorbent	80 - 95	80	X	X	X
membrane separation	<99	80	Z	Z	Z
biofiltration	75 - 95	75	Z	Z	Z
cold oxidation	80 - >99.9	80	Z	Z	Z
air filtration	70 - 99	70	Z	X	Z

X – abatement technology broadly applicable

Z – abatement technology may be applicable

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.

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

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

The preceding list of air treatment technologies is not exhaustive; others may exist that are capable of capturing volatiles and ameliorating the air emission profile. These include technologies such as cryo-condensation, 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 where there is no application of WTP sludge to agricultural soil or arable land (ECHA, 2016). It is also understood that good housekeeping and maintenance procedures are in place to minimize the potential for soil release. Aside from these requirements, there are no discretionary risk management measures that may be instituted to minimize the release of volatile substances to soil (CEFIC, 2007).

5. Exposure assessment input

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

5.1. Substance use rate

The three SpERCs identified in this guidance document have dissimilar maximum estimated usage rates that reflect differences in the handling capacities at alternative stages of the life cycle (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 default value of 300. 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 associated with the three SpERCs described herein.

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

Tonnage	SpERC title		
	manufacture	formulation	intermediate
Local use rate (kg/day)	2,000,000	100,000	50,000
Emission days	300	300	300
Fractional local EU tonnage	100%	100%	100%
Fractional regional EU tonnage	100%	100%	100%
Rationale	tanker truck shipments	published citation	tanker truck shipments

* Local and regional tonnages are applied to life cycle stages where wide dispersive uses occur.

The estimated local use rate for manufacturing and use as an intermediate were based on professional judgement and take into consideration the number of tanker trucks that a facility is typically capable of handling each 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 loaded tanker trucks processed at a site was conservatively estimated to be 80 per day for a manufacturing, 2 per day for use as a processing aid, and 2 per day for use as an intermediate. The equation used to calculate these use rates is as follows:

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

The local use rate for the formulation SpERC was derived using published information on the production capacity of major automotive and specialty lubricant manufacturers operating in the United Kingdom (OECD, 2004). The upper size limit for a typical facility formulating specialty lubricants as their sole product was reported to be 30,000 tonnes/year, which is equivalent to 100,000 kg/day for a site operating 300 days/year. The equation used to calculate the formulation use rate is as follows:

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

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 is the same for each of the SpERCs described in this guidance document (see Table 3). The value of 300 days/year is the default value for substances manufactured in an amount greater than 10,000 tonnes/year; formulated in an amount greater than 2,000 tonnes/year, or used at an industrial site in an amount greater than 5,000 tonnes/year (ECHA, 2016). The tonnage cut-off limits cited above represent the maximum worst-case 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 is directly impacted by both 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, five water solubility categories and 4-6 vapour pressure categories were identified. Although this approach resulted in the creation of a large number of sub-SpERCs, it also provided a more precise scheme for assigning a release factor to a particular volatile solvent.

a) Release factor to air

The release factors to air have been adopted from an authoritative source that describes the air emission profiles for a host of basic chemicals such as solvents and other primary chemical intermediates obtained during the crude oil refining process (EC, 2003). A total of 17 Industrial Categories (ICs) have been established for classifying the sectors of use for a particular volatile substance (OECD, 2003). The ICs and their associated applicability domains are presented in Appendix 1. The use characteristics of a substance have been further refined using six Main Categories (MCs) in conjunction with a description of the relevant life cycle stage. Table 4 describes the individual MCs and the use patterns that characterizes each designation (EC, 2003). This segregation scheme was created to allowed emission experts to assign air release factors to a substance depending on its volatility and overall pattern of use.

Table 4. Use pattern associated with individual main category codes for different stages of the life-cycle.

Main Category	Life-cycle stage	Interpretation
Ia	Production	Non-isolated intermediates
Ib	Production	Isolated intermediates stored on-site, or substances other than intermediates produced in a continuous production process
Ib	Formulation	Dedicated equipment and (very) little cleaning operations
Ic	Production	Isolated intermediates stored off-site, or substances other than intermediates produced in dedicated equipment
Ic	Formulation	Dedicated equipment and frequent cleaning operations
II	Formulation	Inclusion into or onto a matrix
II	Industrial/ Professional	Non-dispersive use (industrial point sources), or processing of intermediates in multi-purpose equipment
III	Production	Multi-purpose equipment
III	Formulation	Multi-purpose equipment
III	Industrial/ Professional	Non-dispersive use (industrial point sources), or processing of intermediates in multi-purpose equipment
IV	Industrial/ Professional	Wide dispersive use (many small point sources or diffuse releases; normally no emission reduction measures)

The information in Tables 4 allowed the use characteristics to be identified for each of the SpERCs described in this background document. The compiled information, listed in Table 5, allowed identification of the appropriate A-Table, which lists the air release factor as function of solvent volatility. This process yielded the compilation of air release factors presented in Table 6.

The air emission factors shown in Table 6 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 accomplished using the following formula:

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

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

Identifiers	SpERC title		
	manufacture	formulation	intermediate
Industry category	IC=2 Chemical industry (basic chemicals)	IC=2 Chemical industry (basic chemicals)	IC=3 Chemical industry (intermediates)
Main category	III Non-dispersive industrial use or processing of intermediates	III Non-dispersive industrial use or processing of intermediates	Ic Isolated intermediates stored off-site or other substances produced in dedicated equipment
Use category	48 (solvents)	48 (solvents)	33 (intermediates)
A-table number	A1.1	A2.1	A1.2

Table 6. SpERC air release factors for each vapour pressure category

Vapour pressure (Pa)	SpERC air release factor (%)		
	manufacture	formulation	intermediate
>10000	5.0	NA	2.5
>1000	NA	2.5	NA
1000-10000	5.0	NA	1.0
100-1000	1.0	1.0	0.1
10-100	0.1	0.5	0.01
1-10	0.01	NA	0.0001
<10	NA	0.25	NA
<1	0.001	NA	0.000

NA – not applicable

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., m³ wastewater/tonne solvent produced) needs to be known. Using this information, the water release factor can be calculated using the following formula:

$$\text{Release factor (\%)} = \frac{\text{wastewater volume} \left(\frac{\text{m}^3}{\text{tonne}} \right) \times \text{water solubility} \left(\frac{\text{mg}}{\text{L}} \right) \times 1000 \left(\frac{\text{L}}{\text{m}^3} \right)}{1.0 \times 10^9 \left(\frac{\text{mg}}{\text{tonne}} \right)} \quad (4)$$

The release factors to water were 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 the production capacity. These sources are individually highlighted below.

1. Surveys of wastewater generation at approximately 100 European oil refineries have documented effluent release volumes per tonne of refinery output (CONCAWE, 2012). Three surveys conducted in 2005, 2008, and 2010 found average effluent volumes of 1.2, 0.82, and 0.56 m³/tonne, respectively. These data were used to establish a cautiously representative estimate of wastewater generation for the manufacture and intermediate SpERCs. A value of 10 m³/tonne of solvent produced or processed was consistent with the results from the refinery surveys and adequately accounted for the margin of error in the reported values.
2. Wastewater generation for the formulation SpERC was assessed separately using published information from an emission scenario document (ESD). The aqueous discharge from a blending plant involved with the formulation of industrial purpose lubricating oils was stated to be 100 L/tonne (0.1 m³/tonne) (OECD, 2004). Based on this reporting, wastewater discharge volume of 5 m³/tonne was judged to provide a suitably conservative estimate for calculating the water release factors associated with the formulation SpERC.

Using these data, the water release factors listed in Table 7 were calculated for the three 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.

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

Water solubility (mg/L)	SpERC water release factor (%)		
	manufacture	formulation	intermediate
<1	0.001	0.0005	0.001
1-10	0.003	0.002	0.003
10-100	0.03	0.02	0.03
100-1000	0.3	0.2	0.3
>1000	1.0	0.5	1.0

c) Release Factor - soil

The SpERC-related soil release factors have been compiled from several different sources. As shown in Table 8, values of 0.01 or 0.1 have been assigned using ECHA-reported default assignments (ECHA, 2016). The ECHA default values have been conservatively estimated and assume that some soil release will occur as a result of the spillage that may accompany the transfer or delivery of materials or when equipment leaks develop in pumps, pipes, reactors, and storage tanks. In addition, the soil release factors take into consideration the wet and dry soil deposition that may accompany the airborne release of a volatile substance. The factors have been cited with the understanding that some release to soil may occur during equipment upsets. In addition, the supplied soil release factor takes into consideration the wet and dry soil deposition that may accompany the airborne release of a volatile substance. Soil releases from these situations are not expected to be a common occurrence because a majority of the operations covered by these SpERCs take place indoors.

Table 8. SpERC soil release factors and their associated ERC value

Assignments	SpERC title		
	manufacture	formulation	intermediate
ERC	1	2	6a
Release factor (%)	0.01	0.01	0.1
Source	(ECHA, 2016)	(ECHA, 2016)	(ECHA, 2016)

d) Release Factor – waste

A thorough and detailed analysis accompanied the determination of waste release factors for the three SpERCs outlined in this background document. Although a substantial amount of information is available that documents the total amount of different waste types produced annually by solvent producers or 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, in some cases, 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. Industrial surveys of waste generation and authoritative reviews of waste handling practices also provide potentially useful sources of information on the production of different waste types.

The waste factors provided in Table 9 are focused on the production of solvent-containing by-products and residues that have no further use and need to be disposed of in a conscientious manner (Inglezakis and Zorpas, 2011). Refineries and their associated petrochemical facilities are 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 by-products and residues (EEA, 2016).

Table 9 provides a listing of the waste generation factors and their associated literature sources for each of the three SpERCs under consideration.

Table 9. SpERC waste release factors and their literature source

Assignments	SpERC title		
	manufacture	formulation	intermediate
Release factor (%)	0.2	4.0	5.0
Source	(CONCAWE, 2017)	(Yilmaz, 2006)	(EC, 2017a)

1. Manufacture

The types of waste generated during the manufacture of solvents in European petrochemical facilities has been reliably assessed and reported upon. A 2015 survey of waste production at 104 European refineries yielded some important insights and allowed a waste release factor to be assigned to manufacturing operations (CONCAWE, 2017). The survey asked respondents to provide quantitative waste generation and waste management information for 35 individual waste categories that included organic solvents. The responses from 77 refineries showed that the generation of hazardous waste during refinery operations averaged 1.07 tonne/kilotonne and ranged from 0.44 to 1.99 tonnes/kilotonne of manufactured product. This is equivalent to an average waste release factor of 0.11% that ranged as high as 0.20%. A majority of this hazardous waste was found to be composed of tank bottom and wastewater treatment sludges generated during normal refinery operations. On the basis of this survey information, the waste release factor for manufacturing was conservatively set at the upper limit value of 0.2% recognizing that the true value may be considerably less.

2. Formulation

The waste generation value associated with solvent formulation and handling was based on published reports of the hazardous waste resulting from the commercial preparation of vinyl chloride monomer (VCM) at facilities in Turkey and India. A site in Turkey producing 140,580 tonnes/yr of VCM created 3,500 – 5,600 tonnes/yr of liquid hazardous waste (Yilmaz, 2006). This is equivalent to a waste generation factor ranging

from 2.5 – 4.0%. A separate facility in India reported the creation of 4.1 kg/tonne (0.41%) of reactor waste, viscous bottom waste, surge pond sludge, and carbon waste during VCM production (UNEP, 2014). A waste generation factor at the upper range of these reported values was judged to be a suitably cautious estimate of the hazardous waste generation potential for a wide array of formulation activities.

3. Intermediate use

A recent BREF (Best Available Techniques Reference Document) for the production of large volume organic chemicals provides a useful synopsis of the amounts and types of waste associated with the production of oxygen-containing hydrocarbon solvents from specific chemical precursors (EC, 2017a). Waste resulting from the production of 2-ethylhexanol from butyraldehyde in a multi-step process involving aldol condensation and hydrogenation was reported to be less than 50 kg/tonne of product, which yields a waste generation factor of 5% or less. This limit value provides a broadly applicable ceiling for the hazardous wastes generated when solvents are used as chemical intermediates.

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:

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

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:

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

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

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

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:

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

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.

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

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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Appendix 1

Table A1. Industrial categories and their overall scope

Industrial Category Code	Title	Description
IC 0	Others	Includes all processes and activities, which cannot be placed in one of the following industrial categories. An example is food processing industry.
IC 1	Agricultural Industry	Activities involving the growing crops and the raising cattle. It also comprises all allied activities such as pest control and manure handling.
IC 2	Chemical industry: basic chemicals	Covers chemical production using raw materials from the petrochemical industry, from plant and animal materials, or coal. The category is dedicated to basic chemicals, which are substances used generally throughout all branches of chemical industry and usually in considerable amounts.
IC 3	Chemical industry: chemicals used in synthesis	Chemicals used in synthesis are substances either regulating the chemical reaction process (e.g. catalysts) or being used as an intermediate (i.e. chemicals that can be isolated at an intermediate step between starting material and the final product).
IC 4	Electrical/electronic industry	Manufacture of components like resistors, transistors, capacitors, diodes, lamps, and the production of televisions, radios, computers (PC's as well as mainframes), radar installations, and complete telephone exchanges. Processes include electroplating, polymer processing, and paint application.
IC 5	Personal/domestic	Includes the use and application of substances in the home for maintenance and care of houses, furniture, kitchenware, gardens, and personal care (hygiene and make-up). Chemicals used in this category will often be present in formulations (e.g. in cleaners such as soaps, detergents, and washing powders, cosmetics, and products for the care of leather, textile and automobiles).
IC 6	Public domain	Covers the application and use of substances in a variety of places by skilled workers. Sites include offices, public buildings, waiting rooms, various workshops like garages. Activities include the professional cleaning and maintenance of buildings, streets, and parks. Most substances will exist as formulations, (e.g. cleaners, non-agricultural biocides and products for the maintenance of roads and buildings).
IC 7	Leather processing industry	Includes industries where leather is made out of raw hides, where leather is dyed and where products are made out of leather (e.g. shoe manufacture).
IC 8	Metal extraction, refining and processing industry	Covers the extraction of metals from ores, the manufacture of primary/secondary steel and non-ferro metals as well "pure" alloy metals, and the various metal shaping and working processes like cutting, drilling, and rolling.
IC 9	Mineral oil and fuel industry	Includes the petrochemical industry, which processes crude mineral oil. By means of physical and chemical processes (e.g. separation by means of distillation, cracking and platforming) they produce a wide range of hydrocarbons serving as raw materials for chemical industry and (often after adding a series of additives) fuels for heating and combustion engines.
IC 10	Photographic industry	Consists of the manufacture of photographic materials such as film and photographic paper. Includes the production of solid and liquid preparations for film and paper processing. Printshop operations and processing of films and photographic paper is also considered.
IC 11	Polymers industry	Comprises a branch of the chemical industry where thermoplastics are produced or processed by means of a wide range of techniques.
IC 12	Pulp, paper and board industry	Includes the production of pulp, paper and cardboard out of wood or waste paper. Also incorporates those chemicals used in reprographic industry.

IC 13	Textile processing industry	Covers the cleaning, spinning, and dyeing, of fibre as well as weaving and finishing (e.g. impregnation and coating) operations.
IC 14	Paints, lacquers and varnishes industry	Includes the manufacture, formulation, and application of coating products.
IC 16	Engineering industry: civil and mechanical	Comprises of industrial activities associated with wood processing (e.g. wooden furniture), motor car manufacturing, and building construction.