# ESIG/ESVOC SpERC
# Background Document

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

European Solvents Industry Group (ESIG)
European Solvents Downstream Users Coordination Group (ESVOC)
Avenue E. van Nieuwenhuyse 4
1160 – Brussels Belgium
esig@cefic.be

**Introduction**

Petrochemicals comprise a large group of volatile substances that can include the end products from crude oil refining as well as the chemical substances obtained from the downstream conversion hydrocarbon feedstocks. These substances may be 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 volatile hydrocarbon in a particular application is dictated, in part, by its physical and chemical properties, which can vary over a very broad range. They may also be used in combination when specific chemical characteristics are needed for a particular process or product.

Chemical emissions can take place during multiple life cycle stages including production, storage, transport, and use. Air, water, and soil release will occur 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 corresponding SpERC factsheet and provide additional descriptive details on the genesis and informational resources used to generate each SpERC.

## 1. Title

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

1. ESVOC SPERC 4.10a.v4 – Use as binders or release agents
2. ESVOC SPERC 4.3a.v4 – Use in coatings
3. ESVOC SPERC 4.4a.v2 – Use in cleaning agents
4. ESVOC SPERC 4.7a.v2 – Use in metalworking fluids/rolling oils

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

## 2. Scope

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

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

Figure 1. ECHA identified life cycle stages and their interrelationship

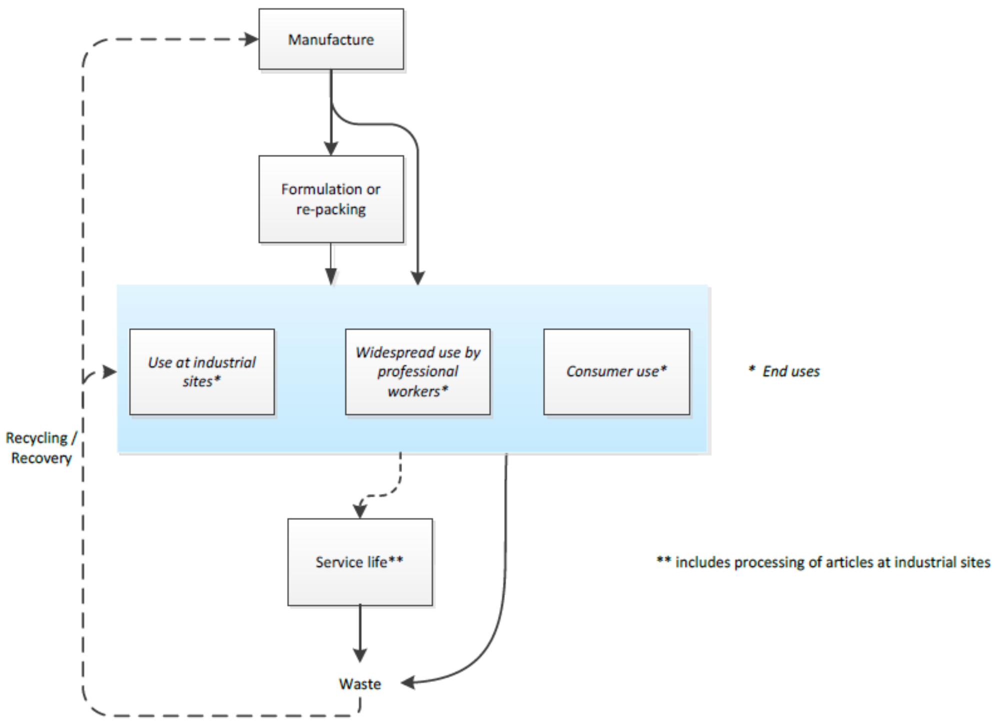

Table 1. SpERC background information

| SpERC Code | Title | Life Cycle Stage (LCS) | Sector of Use (SU) | Chemical Products Category (PC) | Use Description |
|---|---|---|---|---|---|
| ESVOC SPERC 4.10a.v4 | Use as binders or release agents | Industrial end-use | SU0 other | PC24 lubricants, greases, release products | Covers the use as binders and release agents including material transfers, mixing, application (including spraying and brushing), mould forming and casting, and handling of waste. |
| ESVOC SPERC 4.3a.v4 | Use in coatings | Industrial end-use | SU0 other | PC9a coatings and paints, thinners, paint removers | Covers the use in coatings (paints, inks, adhesives, etc.) including exposures during use (including materials receipt, storage, preparation and transfer from bulk and semi-bulk, application by spray, roller, spreader, dip, flow, fluidized bed on production lines and film formation) and equipment cleaning, maintenance and associated laboratory activities. |
| ESVOC SPERC 4.4a.v2 | Use in cleaning agents | Industrial end-use | SU9 other | PC35 washing and cleaning products | Covers the use as a component of cleaning products including transfer from storage, pouring/unloading from drums or containers. Exposures during mixing/diluting in the preparatory phase and cleaning activities (including spraying, brushing, dipping, wiping, automated and by hand), related equipment cleaning and maintenance. |
| ESVOC SPERC 4.7a.v2 | Use in metal working fluids/rolling oils | Industrial end-use | SU9 other | PC25 metal working fluids | Covers the use in formulated MWFs/rolling oils including transfer operations, rolling and annealing activities, cutting/machining activities, automated and manual application of corrosion protections (including brushing, dipping and spraying), equipment maintenance, draining and disposal of waste oils. |

## 3. Operational conditions

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

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

Biological wastewater treatment (WWT) may involve the use of both industrial and municipal treatment facilities. 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 chemical products for use in a multitude 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 organic chemicals 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 substance 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 products 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 chemical substance 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, 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 organic chemicals 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 are described in Table 2 along with the range of measured removal efficiencies, the assigned nominal removal efficiency to be applied when adjusting an air emission factor, and the SpERCs where the technology may be applicable.

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

| Air abatement technology | Reported abatement efficiency range (%) | Assigned abatement efficiency (%) | Applicability to individual SpERCs | | | |
|---|---|---|---|---|---|---|
| | | | ESVOC SPERC 4.10a.v4 | ESVOC SPERC 4.3a.v4 | ESVOC SPERC 4.4a.v2 | ESVOC SPERC 4.7a.v2 |
| wet scrubbers | 50 - 99 | 70 | Z | X | X | Z |
| thermal oxidation | 95 - 99.9 | 95 | X | X | X | X |
| solid adsorbent | 80 - 95 | 80 | X | X | X | X |
| membrane separation | <99 | 80 | Z | Z | Z | Z |
| biofiltration | 75 - 95 | 75 | Z | Z | Z | Z |
| cold oxidation | 80 - >99.9 | 80 | Z | Z | Z | Z |
| air filtration | 70 - 99 | 70 | Z | X | Z | X |

X – abatement technology broadly applicable

Z – abatement technology may be applicable

The treatment technologies include wet scrubbers, thermal oxidation, vapour adsorption, membrane separation, biofiltration, cold oxidation, and air filtration (EC, 2016, Schenk, et al., 2009). The range of removal efficiencies cited in Table 2 reflect the variability that has been reported in a BREF (BAT Reference) document. The VOC removal efficiency of wet scrubbers is notable because of the large range in reported values. This variability is due in part to differences in the plant configuration, equipment operating conditions, and the type of VOC examined. An examination of the BREF reported values from three separate wet scrubber field studies suggests the use of a nominal abatement efficiency value of 70%, which was judged to be representative of the typical removal efficiency of wet scrubbers for solvent volatiles. The rationale stems from observed removal efficiencies of 70% or greater in two of the three reported studies. Similarly, the abatement efficiency of thermal oxidizers was reported 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 to greater than 99%. Higher removal efficiencies may be applied when any of these technologies are used in combination within a vapor recovery unit. Air filtration techniques such as wet dust scrubbing may be used to remove soluble particulate matter, aerosols, and mist from an airstream. The removal efficiencies attainable with these methods varies depending the type of scrubber being used, with reductions of 70 - 99% observed with a fibrous packing scrubber using glass, plastic, or steel packing material.

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

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

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

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

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

## 5. Exposure assessment input

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

### 5.1. Substance use rate

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

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

| Tonnage | SpERC title | | | |
|---|---|---|---|---|
| | ESVOC SPERC 4.10a.v4 | ESVOC SPERC 4.3a.v4 | ESVOC SPERC 4.4a.v2 | ESVOC SPERC 4.7a.v2 |
| Local use rate (kg/day) | 25,000 | 50,000 | 5,000 | 25,000 |
| Emission days | 100 | 300 | 20 | 20 |
| Fractional local EU tonnage | 100% | 100% | 100% | 100% |
| Fractional regional EU tonnage | 100% | 100% | 100% | 100% |
| Rationale | tanker truck shipments | tanker truck shipments | tanker truck shipments | published citation |

The estimated local use rate at sites manufacturing binders/release agents, coatings, and cleaning agents were based on professional judgement and take into consideration the number of tanker trucks that are off-loaded at a representative facility per day. These tankers are assumed to operate in accordance with EU Directive 96/53/EC governing the maximum authorized weights and dimensions of road trailers in Europe (EU, 1996). In agreement with the legislation, the payload capacity of the transport vehicles is presumed to be 25 metric tons (Znidaric, 2015). The number of off-loaded tanker trucks processed at a site was conservatively estimated to be 1 per day for the use in the production of binders/release agents, 1 per week (assuming a 5-day work week) for the formulation of cleaning agents, and 2 per day for use in coating preparations. The equation used to calculate these use rates is as follows:

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

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

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

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

### 5.2. Days emitting

The number of emission days for each of the SpERCs described in this guidance document vary as shown in Table 3. The value of 300 days/year is the default value for substances used in industrial applications in an amount greater than 5,000 tonnes/year; whereas the value of 100 days is applicable to operations where the use amounts are greater than 1,000 tonnes/year and less than 5,000 tonnes/year. A value of 20 days/year is applied when the industrial use if less than 1,000 tonnes/year (ECHA, 2016). The tonnage cut-off limits cited above represent the maximum use amount at a single site.

### 5.3. Release factors

The magnitude of an environmental emission following the production or use of an organic chemical 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 chemical substances found in commerce, a single emission factor does not adequately portray the release of all the chemicals in a particular 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 substances with high water solubility or volatility to be distinguished from those with a low to intermediate values. Using this approach, 8 water solubility categories and 4-6 vapour pressure categories were created. Although this scheme 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 petrochemical substance.

#### *1. Release factors to air*

A variety of resources were tapped to derive air release factors for the four industrial use categories considered herein. These include both published and unpublished reports from authoritative sources as well as informed experts knowledgeable of the processes and procedures associated with a particular industrial application. When reliable information was unavailable for a stated industrial use, a worst-case default estimate was applied.

Otherwise, the listed air release factors were adopted once the information was suitably vetted.

A. Use in releasing agents and binders

The A-tables of Appendix 1 in the Technical Guidance Document (TGD) on Risk Assessment Part II provided the information needed to establish air release factors for this SpERC (EC, 2003). Although the use of binders and release agents is not explicitly described in any of the 16 industrial categories evaluated in the TGD, the use can be assigned to the "Others" category, which is used for emission sources that are not covered by an explicitly defined industrial category. Industrial usages placed in the "Others" industrial category are may be evaluated using the air emission factors described in Table A3.16. This A-table is unlike many others since it stratifies the release factors according to both water solubility and vapor pressure, which leads to the creation of an unusually large number of choices. Since the mineral oils, waxes, and hydrocarbons used use as die casting release agent lubricants are all characterized by their low water solubility, the air release factors associated with substances having a water solubility less than 100 mg/L were deemed to be the most relevant for the binder and release factor use category (Kiteley and Hunt, 1970). The air release factors cited in Table 5 have therefore been assigned using the following use characteristics.

| | |
|---|---|
| Industry category | IC=0 (Others) |
| Main category | III (Non-dispersive industrial use) |
| Use category | 6 (Anti-set-off and anti-adhesive agents) |
| A-table number | A3.16 (associated with IC=16; Engineering industry: civil and mechanical) |

B. Use in coatings

The air release factor associated with the use of coatings was based on field measurements provided in an OECD Emission Scenario Document (OECD, 2015). The monthly release of volatiles associated with the industrial application of water and solvent-based coating to new car bodies was reported to be 43 g/m$^2$. Using the stated monthly output of 200,000 m$^2$ of coated metal surface, this value is equivalent to an emission mass of 8.6 metric tons. The total monthly usage of automotive coatings at the paint plant was stated to be 43.3 tonnes and the average volatile content of the coatings was determined to be 37%. These values yield a monthly VOC usage amount of 16 tonnes and a resulting air release factor of 54% (8.6/16 X 100). This factor provides a reasonable real-world estimate of the air emissions that would be expected when a coating is used in a high-volume industrial application.

Consequently, no upward adjustments or modifications are needed to address coating usage in other industrial applications where there is a potential for release.

C. Use in cleaning agents

The ERC 4 default value of 98% has been adopted since factual information describing the actual air emission value is unavailable (ECHA, 2016). The listed default value has been attributed to the use of non-reactive processing aid at industrial site (no inclusion into or onto article). Processing aids include the use of solvents in cleaners, paints, adhesives and other products. The genesis of this value reportedly stems from an examination of the release factors posted in the A-Tables of Appendix 1 in the Technical Guidance Document (TGD) on Risk Assessment Part II (EC, 2003).

D. Use in metalworking fluids

An air release factor of 2% as been assigned to the SpERC for metalworking fluid use. Justification for this value stems from an examination of the emissions resulting from the use of neat oils in metal machine shops (OECD, 2004). Evaporation of volatile components was not expected to be high due to the low volatility of the various components at room temperature.

Table 5. SpERC release factors for air

| **Vapour pressure (Pa)** | **SpERC title** | | | |
|---|---|---|---|---|
| | **Binders/ release agents** | **Coatings** | **Cleaners** | **Metalworking fluids** |
| >10,000 | **75** | See text below | See text below | See text below |
| 1000-10,000 | 50 | | | |
| 100-1000 | 10 | | | |
| 10-100 | 1 | | | |
| <10 | 0.1 | | | |

The preceding air emission factors 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.

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

$$Release\ factor\ (\%) = \frac{wastewater\ volume\ \left(\frac{m^3}{tonne}\right) \times water\ solubility\ \left(\frac{mg}{L}\right) \times 1000\ \left(\frac{L}{m^3}\right)}{1.0\times10^9\ \left(\frac{mg}{tonne}\right)} \qquad (4)$$

This allows the water release factors to be calculated for eight 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. If specific knowledge is available on the water solubility of the chemical substances being used in a particular application, the release factors may be adjusted to account for the difference between the actual and nominal water solubility values.

In some cases, a reasonable and definitive information could not be located in the scientific literature. In these cases, the absence of information was offset using expert professional judgement and industry sector knowledge acquired by a variety of means including networking opportunities, trade association meetings, and social media interactions.

#### A. Use in releasing agents and binders

A literature review identified a single reliable determination of release agent and water use volumes for an aluminum die casting plant manufacturing parts for the automotive industry (Neto, et al., 2008). Release agent usage during casting operations was reported to be 10.5 L/tonne alloy used, whereas the water usage was listed at 1.03 $m^3$/tonne alloy. Assuming a release agent density of 1.0 kg/L, these values yield a water use factor of 98 $m^3$/tonne agent (1.03/10.5*1000). The updated value was used to calculate the water release factors that are listed in Table 6.

B. Use in coatings

A wastewater generation factor was determined using the information compiled in a life cycle analysis of spray-painting operations at a North American motor vehicle assembly plant (Anastassopoulos, et al., 2009). The total VOC content of the applied coats of primer and topcoat were reported to be 6.52 and 9.05 kg per 1000 $m^2$ of body surface area respectively. The volume of wastewater from the painting operation was reported to be 6.87 $m^3$ per 1000 $m^2$ of automotive body surface area. The ratio of the wastewater volume of 6.87 $m^3$ to the total paint VOC usage rate of 0.016 tonnes (primer plus topcoat) yields a wastewater generation factor of 441 $m^3$ of wastewater per tonne of VOC. When the value was substituted into the above equation, it yielded the water release factors identified in Table 6.

C. Use in cleaning agents

In some cases, a reasonable and definitive information database could not be located in the scientific literature. The absence of information was offset using expert professional judgement and industry sector knowledge acquired by a variety of means including networking opportunities, trade association meetings, and social media interactions. Sector knowledge was vital in establishing the wastewater generation volumes associated with the industrial use of cleaning agents. Using this approach, a function wastewater generation volume of 0.1 $m^3$/tonne was estimated to apply. Substituting this value into the release factor equation allowed the determination of the five factors shown in Table 6.

D. Use in metalworking fluids

Wastewater generation for the coating and metalworking fluid SpERCs was assessed using published information from the scientific or technical literature. The aqueous discharge associated with the blending of a metalworking fluid was assessed for a UK site producing 10,000 tonnes of lubricant per year (OECD, 2004). The wastewater discharge volume for this site was stated to be 100 L/tonne (0.1 m3/tonne). To account for any uncertainties in the reporting and to ensure an adequate margin of environmental protection, a 10-fold adjustment factor was applied to the reported value. This adjustment yielded a wastewater generation volume of 1.0 $m^3$/tonne, which allowed the calculation of the five release factors shown in Table 6 for the use of metalworking fluids.

Table 6. SpERC water release factors for each water solubility category

| Water solubility (mg/L) | SpERC water release factor (%) | | | |
|---|---|---|---|---|
| | Binders/ release agents | Coatings | Cleaners | Metalworking fluids |
| <0.001 | 1 x $10^{-7}$ | 0.00004 | --- | --- |
| 0.001-0.01 | 0.00003 | 0.0001 | --- | --- |
| 0.01-0.1 | 0.0003 | 0.001 | --- | --- |
| 0.1-1 | 0.003 | 0.01 | --- | --- |
| <1 | --- | --- | 0.00001 | 0.0001 |
| 1-10 | 0.03 | 0.1 | 0.00003 | 0.0003 |
| 10-100 | 0.3 | 1 | 0.0003 | 0.003 |
| 100-1000 | 3 | 14 | 0.003 | 0.03 |
| >1000 | 10 | 44 | 0.01 | 0.1 |

### 3. *Release factors to soil*

The SpERC-related soil release factors have been compiled from several different sources. As shown in Table 7, a value of zero or one has been assigned using ECHA-reported default assessments, professional judgement and available sector knowledge, or published OECD emission scenario information.

A. Use in releasing agents and binders

The value was derived from information contained in the same A-table used to establish the air release factors for binders and release agents. This is the A-table identified for use with industrial processes that do fit neatly withing one of the 16 categories described in the EU Technical Guidance Document on Risk Assessment and are therefore placed in the "Others" (IC=0) Category (EC, 2003). The TGD document indicates that industrial processes in the "Others" category can reference the soil release factors in Table A3.16 which is aligned with civil and mechanical engineering industry (IC=16).

The soil release factors in table A3.16 cover a range of water solubilities and vapor pressures. The values for production stage MC III which includes substances that are not widely dispersed range from 0 to 1.0%. To ensure that substances of very low water solubility (i.e., <100 mg/L) and vapor pressure (i.e., <10 Pa) are captured, the highest soil release factor of 1.0% is advocated for use with the binder and release agent SpERC. Use of this value ensures that the soil release potential of all binders and release agent constituents have been considered and that an adequate degree of precautionary diligence has been introduced into the process.

B. Use in coatings

The OECD emission scenario document for coating application considers the soil releases associated with the painting of new and refurbished vehicles (OECD, 2009). The analysis finds that the painting of new vehicles is not associated with any substantial opportunity for the release of organics to soil. In contrast, the refinishing of existing vehicles was associated with a small but measurable release to soils that came with the equipment cleaning. This release, however, was confined to solids and not organics. Similarly, the industrial application of coatings to metal packaging cans and various sheet metal products used in appliance manufacturing and building construction were also devoid of any notable release to soil. These data support using a soil release factor of zero for the industrial use of coatings.

C. Use in cleaning agents

The soil release value for cleaning agents has been conservatively estimated with the understanding that very small releases to soil may occur in some instances. These include the spillages that may accompany transfer or delivery and the development of leaks in pumps, pipes, and storage tanks. The soil affected by minor spills is often promptly attended to and the area decontaminated to ensure that there is no residual release. Since a majority of the operations covered by the cleaning SpERC takes place indoors, soil spills are not expected to be a common occurrence. As such, a release factor of zero can be confidently applied.

D. Use in metalworking fluids

An examination of the environmental releases of associated with the use of metalworking and cutting fluids failed to show a measurable release of these products to soil during the blending process (OECD, 2004). Consequently, a factor of zero has been assigned for use of these fluids in all industrial applications.

Table 7. SpERC release factors for soil

| Assignments | SpERC title | | | |
|---|---|---|---|---|
| | **release agent use** | **coating use** | **cleaner use** | **metalworking fluid use** |
| ERC | 4 | 4 | 4 | 4 |
| Soil release factor (%) | 1 | 0 | 0 | 0 |
| Source | (EC, 2003) | (OECD, 2009) | professional judgement | (OECD, 2004) |

### 4. *Release factors to waste*

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

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

Three of the four waste release factors cited in Table 8 have been derived from published life cycle assessments (LCAs) that inventory the emissions and wastes generated during the different stages of a product's service life. These values may be used in the absence of detailed information for a particular industrial operation. These generic values may be supplanted if the actual hazardous waste generation factor is known for the industrial operation under consideration. To guarantee that an adequate margin of protection was built into the determination, an adjustment factor of 10 has occasionally been applied when a reported value was judged to be unrepresentative for the entire range of potential use conditions within a particular industrial sector.

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

Unlike the preceding SpERCs, the waste release factor for the use of solvents in the preparation of coating formulations was taken from an ESD (OECD, 2009). A waste release factor of 0.5% was calculated to be indicative of the residues generated during the batch production of an organic solvent-borne coating. Although the preceding release factors are reasonably indicative of the hazardous waste generation potential in each of the targeted industry sectors, they do not take into consideration the variability associated with using unconventional manufacturing or use practices. The use of a volatile degreasing agent in the metal working industry provided a reasonable estimate of the waste associated with the industrial use of cleaning products (Vollebregt and Terwoert, 1998). The production and use of a mixture of dearomatized C10-C12 hydrocarbons to degrease and treat metal parts was associated with production of 0.4% of solid waste.

Table 8. SpERC waste release factors and their literature source

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

## 6. Wastewater Scaling Principles

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

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

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

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 ($m^3$/day)
$G_{effluent,SPERC}$ – SpERC cited sewage treatment plant flow rate ($m^3$/day)
$q_{site}$ – receiving water dilution factor applicable to the DU site (unitless)
$q_{SPERC}$ – receiving water dilution factor applicable to a SpERC (unitless)

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

Scaling for environmental risk to wastewater treatment plant microorganisms:

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

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

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

*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:*

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

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

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

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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