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 water treatment chemicals, polymers, mining chemicals, and fuels

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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 3.22a.v4 – Use in water treatment
2. ESVOC SPERC 4.21a.v3 – Use in polymer processing
3. ESVOC SPERC 4.23.v3 – Use in mining operations
4. ESVOC SPERC 7.12a.v4 – Use as a fuel

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

2. Scope

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

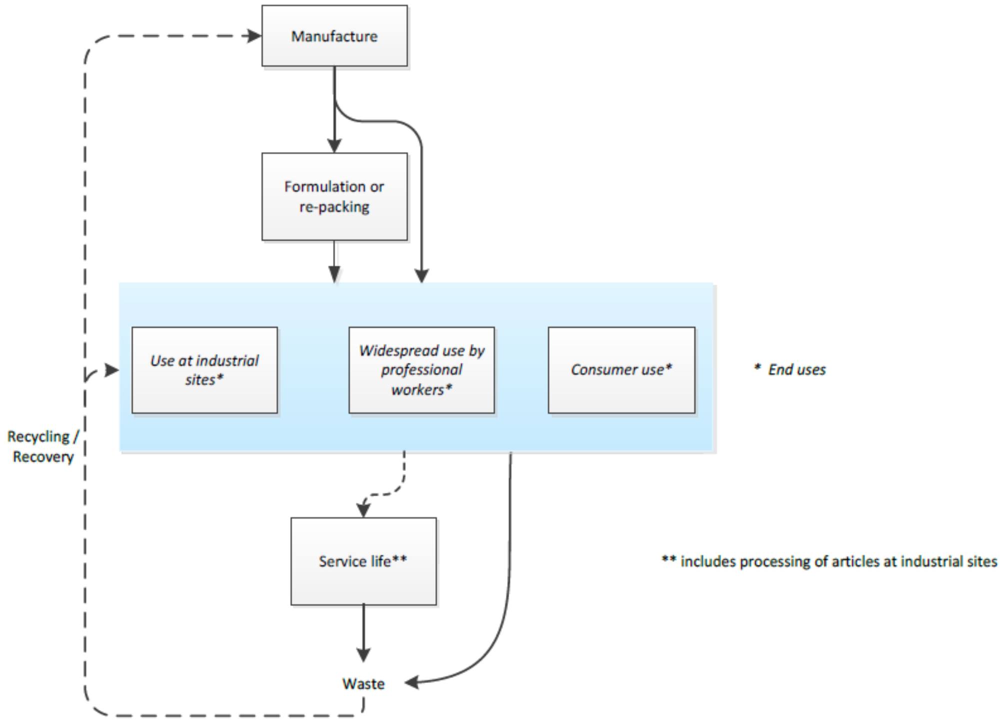

Table 1. SpERC background information

SpERC Code	Title	Life Cycle Stage (LCS)	Sector of Use (SU)	Chemical Products Category (PC)	Use Description
ESVOC SPERC 3.22a.v4	Use in water treatment	Industrial end-use	SU0 other	PC20 processing aids such as pH-regulators, flocculants, precipitants, neutralizing agents	Covers the use of the substance for the treatment of water at industrial facilities in open and closed systems.
ESVOC SPERC 4.21a.v3	Use in polymer processing	Industrial end-use	SU12 manufacture of plastic products, including compounding and conversion	PC32 polymer preparations and compounds	Processing of formulated polymers including material transfers, additives handling (e.g. pigments, stabilisers, and fillers, plasticisers), moulding, curing and forming activities, material re-works, storage and associated maintenance.
ESVOC SPERC 4.23.v3	Use in mining operations	Industrial end-use	SU2a mining (without offshore industries)	PC40 extraction agents	Covers the use of the substance in extraction processes at mining operations, including material transfers, winning and separation activities, and substance recovery and disposal.
ESVOC SPERC 7.12a.v4	Use as a fuel	Industrial end-use	SU8 manufacture of bulk, large scale chemicals (including petroleum products)	PC13 fuels	Covers the use as a fuel (or fuel additive) and includes activities associated with its transfer, use, and equipment maintenance.

3. Operational conditions

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

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

Evidence suggests, however, that municipal WWT plants are not widely used to process industrial wastewaters. This is supported by several surveys of industrial wastewater treatment at European facilities. The first involved a survey of WWT technologies at 81 European chemical facilities that included both large integrated facilities and smaller dedicated stand-alone sites (EC, 2016). The operations at these facilities included the production and formulation of a wide range of chemicals for use in a wide range of downstream applications. The survey results indicated that a majority (i.e. 89%) of the chemical facilities used a dedicated industrial wastewater treatment facility; a much smaller percentage utilized a municipal treatment plant capable of handling both industrial and domestic wastewater. The second survey of industrial operations in Germany found that 4% of the wastewater generated was directed to municipal WWT plants (DECHEMA, 2017). Despite the limited reliance on municipal treatment facilities, their usage is conservatively assumed to exist as a normal operating condition during the downstream use of 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 have been cited in Table 2 along with the range of measured removal efficiencies, the assigned nominal removal efficiency for use when adjusting the assigned air emission factor, and the SpERCs where the technology may be applicable.

The treatment technologies include wet scrubbers, thermal oxidation, vapour adsorption, membrane separation, biofiltration, cold oxidation, and air filtration (EC, 2016, Schenk, et al., 2009). The removal efficiency of wet scrubbers for VOCs can vary depending on the plant configuration, equipment operating conditions, and the type of VOC. The range of removal efficiencies cited in Table 2 reflect the variability that has been 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.

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

Air abatement technology	**Reported abatement efficiency range (%)**	**Assigned abatement efficiency (%)**	**Applicability to individual SpERCs**			
			ESVOC SPERC 3.22a.v4	**ESVOC SPERC 4.21a.v3**	**ESVOC SPERC 4.23.v3**	**ESVOC SPERC 7.12a.v4**
wet scrubbers	50 - 99	70	X	Z	X	Z
thermal oxidation	95 - 99.9	95	X	X	X	X
solid adsorbent	80 - 95	80	Z	X	Z	Z
membrane separation	<99	80	Z	Z	Z	Z
biofiltration	75 - 95	75	Z	Z	Z	Z
cold oxidation	80 - >99.9	80	Z	Z	Z	Z
air filtration	70 - 99	70	Z	Z	Z	Z

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

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

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

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

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

4.3. Optional risk management measures limiting release to soil

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

5. Exposure assessment input

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

5.1. Substance use rate

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

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

Tonnage	**SpERC title**			
	ESVOC SPERC 3.22a.v4	**ESVOC SPERC 4.21a.v3**	**ESVOC SPERC 4.23.v3**	**ESVOC SPERC 7.12a.v4**
Local use rate (kg/day)	100	50,000	10,000	5,000,000
Emission days	300	300	20	300
Fractional local EU tonnage	100%	100%	100%	100%
Fractional regional EU tonnage	100%	100%	100%	100%
Rationale	published citation	tanker truck shipments	tanker truck shipments	published citation

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

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

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

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

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

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

5.2. Days emitting

The number of emission days varies for each of the SpERCs described in this guidance document 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 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. The default value of 20 days/year was not used for the water treatment chemical SpERC, since available sector knowledge revealed that these substances are used on a nearly daily basis.

5.3. Release factors

The magnitude of an environmental emission following the production or use of an organic chemical may be 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 may 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*

In many cases, 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). The EUTGD (European Union Technical Guidance Document on Risk Assessment) lists 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 Table 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.

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

Identifiers	**SpERC title**			
	Water treatment	**Polymer processing**	**Mining**	**Fuels**
Industry category	IC=0 Others	IC=11 Polymers industry	Not applicable	IC=9 Mineral oil and fuel industry
Life cycle stage	Processing	Processing		Processing
Main category	III Non-dispersive industrial use or processing of intermediates	**NA**		III Non-dispersive industrial use or processing of intermediates
Use category	NA	III & IV (solvents and processing aids)		NA
A-table number	A3.16	A3.11		A3.8

NA – not applicable

A. Use in water treatment

A hybrid approach was adopted for the set of air release factors associates with use of water treatment chemicals. Since water treatment chemical did not fit neatly into one of the 16 established industrial categories listed in EUTGD, it was assigned to the "Others" category, which is used when an emission source cannot be easily assigned. Chemical usages placed in the "Others" industrial category requires the use of air emission factors from Appendix Table A3.16, which is aligned with substances used in the Civil and Mechanical Engineering Industry (IC=16). This table is somewhat unique since it takes both water solubility and their vapour pressure into account when assigning an air release factor.

Using these listed factors, the matrix of values shown in Table 6 was created. As shown in the table below the air release factor range from a high of 75% for substances with a vapour pressure greater than 10,000 Pa and a water solubility less than 100 mg/L to a low of 0.001% for materials with a vapour pressure less than 10 Pa and a water solubility greater than 1000 mg/L.

Table 6. Air release factors (%) for water treatment SpERC

Vapour pressure (Pa)	**Water solubility (mg/L)**							
	<0.001	**0.001-0.01**	**0.01-0.1**	**0.1-1.0**	**1-10**	**10-100**	**100-1000**	**>1000**
>10,000	75	75	75	75	75	75	50	10
1000-10,000	50	50	50	50	50	50	10	1
100-1000	10	10	10	10	10	10	5	0.1
10-100	1	1	1	1	1	1	0.1	0.01
<10	0.1	0.1	0.1	0.1	0.1	0.1	0.01	0.001

B. Use in polymer processing

Polymer processing is specifically identified as an industrial category in the EUTGD with the associated air releases listed in Appendix 1 further differentiated according to chemical class and chemical boiling point (EC, 2003). Of the five classes of chemicals identified, two were deemed to be highly relevant to the polymer SpERC: solvents and processing aids.

Category I – additives, pigments and fillers
Category II – plasticizers
Category III – solvents
Category IV – processing aids
Category V – curing and cross-linking agents

The air release factors for class III and IV substances each included a separate group of three factors that could be combined and merged, since they covered differing vapor pressure ranges (solvents: 100 to 10,000 Pa; processing aids: 1 to 100 Pa). Although the processing aid factors were further differentiated according to substance boiling point, the highest and most conservative values applicable to substances with an unknown boiling point were adopted for use. Using this approach, the air release factors listed in Table 7 are recommended for use with the polymer SpERC.

C. Use in mining

An air release factor for mining use was determined using evaporative emission estimates at a copper SX site in southern Arizona (Bishop, et al., 1999). The yearly evaporative losses of six aromatic diluents and other unstated volatiles was determined for settler tanks and a raffinate pond at the site. A total air release rate of 32.3 tonnes per year was determined to occur for the release of all hydrocarbons from all sources. A comparison of the total releases for each individual hydrocarbon showed no obvious relationship with its vapor pressure.

The total air release was further divided by the total reagent usage rate at the SX site to arrive at a release factor. The usage rate at the site was described to be 490,000 gallons per month, which is equivalent to a yearly value of 21,785 tonnes/yr, taking a fuel density of 7.41 lbs/gal into account. This yields an air release factor of 0.15% which was adjusted upward by 25-fold to obtain a conservative estimate that includes the uncontrolled releases that may occur at poorly maintained mining sites. The calculated value of 4% to provides a robust all-inclusive determination of the air releases of volatile chemicals at a mining site.

D. Use as a fuel

The EUTGD specifically lists industrial fuel use as one of its 16 industrial categories. Consequently, the values provide an authoritative and cogent source of information to establish a set of air release factors for industrial use of fuels (EC, 2003) The Mineral Oil and Fuel Industry category A-table list identifies five vapor pressure categories with values ranging from 0.01 to 1.0% for the industrial use life cycle stage. The individual values and associated vapor pressure classes are described further in Table 7 below.

Table 7. SpERC release factors for air

Vapour pressure (Pa)	**SpERC air release factors (%)**			
	water treatment	**polymer processing**	**mining chemical use**	**fuel use**
>10,000	See table above	75	See text above	NA
>1000		NA		1.0
1000-10,000		50		NA
100-1000		25		0.5
10-100		10		0.1
1-10		2.5		0.05
<1		1		0.01

NA – not applicable

The air emission factors shown in Tables 6 and 7 and cited in the text above have not been adjusted for the potential use of an emission abatement device such as those described in section 4.1. Using fractional values, the adjustment is easily calculated using the following formula:

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

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:

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

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 water treatment

Water treatment chemicals can be subdivided into many distinct categories that includes algaecides, biocides, antifoaming agents, coagulants, flocculants, dispersants, surfactants, corrosion inhibitors, pH conditioners, scale inhibitors, and a host of other sequestering agents (Sahu and Chaudhari, 2013). The category containing the largest number of volatile organics are the neutralizing agents which include a number of aliphatic and cycloaliphatic amines that are continually added to boiler water to remove the dissolved carbon dioxide that can lead to acid formation and excessive corrosion. The volatile amines used as neutralizing agents are commonly used in large industrial steam boilers used for power generation. These boilers undergo constant monitoring and maintenance to prevent the accumulation of impurities in the water used for steam generation.

Studies conducted at a Battelle office and laboratory complex composed of 15 separate buildings found that two neutralizing amines (i.e., cyclohexylamine and 2-diethylaminoethanol) were added to the steam boiler feedwater at a rate as high as 1 pound per 40 gallons (Edgerton, et al., 1989). The addition compensated for the amine loss resulting from both the water blowdown and steam release; however, the following data analysis assumes that the addition is entirely related to wastewater blowdown, which provides additional assurance that the determination is sufficiently conservative. Accordingly, the boiler amine addition to the feedwater at the Battelle laboratories can be equated to a wastewater generation factor that can be substituted into the above equation. Using a conversion factors of 4.53×10^{-4} tonne/lb and 3.78×10^{-3} m^3/gallon, the feedwater addition of 40 gal/lb is equal to a metric equivalent of 334 m^3/tonne. When the value of 334 m^3/tonne is substituted into the above equation, it yields the water release factors shown in Table 8 for each water solubility category.

B. Use in polymer processing

Polymer processing can involve molding, curing, and forming activities as well as the handling of additives such as pigments, fillers, stabilizers, and plasticizers. A majority of these polymer additives are non-volatile or of limited water-solubility, so their contribution to the overall emissions profile is relatively minor. The biggest exception, however, is with the plasticizers which can include aromatic, naphthenic, or paraffinic process oils used to alter the properties of a polymer. Process oils are highly complex mixtures of hydrocarbons that are characterized by their color, solubility, volatility, and performance properties (Gedeon and Yenni, 1999). Their biggest use is in the manufacture of thermoplastic elastomers (TPEs) which are rubber-like plastics used to manufacture a variety of automotive, medical, and household products.

A survey of water usage at 16 European TPE manufacturing sites reportedly found a maximum water usage rate of 7 m^3/tonne (EC, 2007). This value included both cooling water and stripping water used to remove excess additives from the freshly blended polymer solutions. Since the authors did not differentiate water usage for each process, the value of 7 m^3/tonne was adopted for use without modification since it was in general agreement with expectations. Its adoption also guaranteed that an adequate degree of conservatism went into the assessment. This value resulted in the list of water release factors shown in Table 6.

C. Use in mining

A wide variety of organic chemicals may be used at mineral mining sites including a range of petroleum-derived hydrocarbons, some with limited solubility and volatility. Perhaps the greatest use of mine chemicals is in solvent extraction where metals are separated and partially purified following initial acid leaching. Solvent extraction (SX) is an important step in the mining of copper, nickel, cobalt, uranium, and many other elements. It involves the treatment of the initial pregnant leach solution (PLS) with a solvent dissolved in a carrier diluent. At some mine sites, this extraction is performed twice to improve copper recovery. The treatment results in the formation of a spent aqueous solution called a raffinate and a variable amount of crud or scum that is composed of an insoluble solid precipitate that contains a sizable amount of organic reagent. The primary and secondary raffinates from the two extraction steps are often handled differently with the primary raffinate sent to a retention pond for recovery and reuse and the secondary raffinate treated as wastewater and sent to neutralization plant (Torralvo, et al., 2017). To ensure an adequate level of conservatism in the release factor determination, both raffinate fractions are being treated as wastewater.

An examination of wastewater streams from a Chilean copper mine reported a raffinate flowrate of 600 m^3/hr or 5,256,000 m^3/yr from the SX plant (Sole, et al., 2016). The wastewater stream contained an entrained organic reagent used to extract copper from the initial leachate. When paired with a determination of the solvent and diluent consumption rate at the SX plant, a suitable wastewater factor can be calculated for use in the above equation. A study of organic reagent use at a large Zambian copper mine reported a maximum consumption rate of 15 kg of solvent and 65 kg of diluent per tonne of copper produced (Sikamo, et al., 2008). This value was annualized using the production volume of copper at the mine, which was quoted to be 200 tonne/day or 73,000 tonne/yr (Ngulube, et al., 2017). This yields a reagent consumption rate of 5,840,000 kg/yr or 5840 tonne/yr. The wastewater generation and reagent consumption rates yield a wastewater generation factor of 900 m^3/tonne (5,256,000 m^3/yr ÷ 5840 tonne/yr). When this value is substituted into the equation above it yields the water release factors shown in Table 8.

D. Use as a fuel

The identification of water release factors for the industrial use of fuels examines the emissions accompanying the use of commercial gas turbines otherwise known as combustion turbines. These units are often used in an industrial setting for either power generation or in mechanical drive applications within the oil and gas industry. Turbine units are capable of running a wide variety of gaseous and liquid fuels including natural gas, refinery gas, kerosene, naphtha, residual oils, heavy distillates, crude oil and others (GE Energy, 2011). This fuel flexibility and the ability to rapidly change over from one fuel type to another is partly responsible for the popularity and wide industrial use of combustion turbines.

The volume of wastewater associated with the use of combustion turbines for power generation is not exceedingly large. The wastewaters generated at facilities using combustion turbines originate from fuel tank dewatering, floor drain washings, sump discharges, oil-water separator releases, as well as cooling water recharges, storm run-offs, filter backwashes, and boiler blowdowns. A permit application for the construction of an electric power plant using three combustion turbines provides usable information on the fuel use and wastewater generation rates accompanying the use of a distillate fuel oil to operate a gas turbine (CSC, 1998). The application indicated that 840,000 gallons of fuel would be needed to operate the three turbines for a period of 18 hours. This is equivalent to 1.12 x 10^6 gallons/day or 4240 m^3/day (i.e., 3519 tonne/day) assuming a distillate fuel oil density of 830 kg/m^3 (Deuker, et al., 2001). The average annual discharge of wastewater from the facility was listed as 55,805 gallons/day or 211 m^3/day. The preceding values provide a highly conservative estimate of wastewater generation since a sizable, but unmeasurable, fraction of the wastewater volume will not come into contact with the hydrocarbon fuel. The ratio of the wastewater generation rate to the fuel use rate yields factor of 0.06 m^3/tonne, which when substituted into the above formula yields the water release factors listed below in Table 8.

Table 8. SpERC water release factors for each solubility category

Water solubility (mg/L)	**SpERC water release factor (%)**			
	water treatment	**polymer processing**	**mining chemical use**	**fuel use**
<0.001	0.00003	7.0 x 10^{-7}	0.0001	6.0 x 10^{-9}
0.001-0.01	0.0001	2.0 x 10^{-6}	0.0003	2.0 x 10^{-8}
0.01-0.1	0.001	0.00002	0.003	2.0 x 10^{-7}
0.1-1	0.01	0.0002	0.03	2.0 x 10^{-6}
1-10	0.1	0.002	0.3	0.00002
10-100	1.0	0.02	3	0.0002
100-1000	10	0.2	30	0.002
>1000	33	0.7	90	0.006

3. *Release factors to soil*

Several sources of information were used to establish a representative soil release factor. This includes values listed in the A-Tables placed inf the Technical Guidance Document on Risk Assessment as well as various published and unpublished descriptions of the soil release accompanying the transfer and use of chemicals in an industrial setting. In some cases, a reasonable and definitive information database could not be located in the scientific literature. The absence of information was counterbalanced using expert professional judgement and industry sector knowledge acquired by a variety of means including networking opportunities, trade association meetings, and social media interactions. These informational resources are described more fully in the following paragraphs and provide the basis for recommending the soil release factors shown below in Table 9.

A. Use in water treatment

A thorough examination of the literature failed to identify any instances where neutralizing amines have been released to soil or groundwater. Likewise, there has not been any reported instances of accidental spills or leakages that have resulted in the contamination of nearby soil or groundwater. These findings indicate that a soil release factor of 0 is both reasonable and appropriate.

B. Use in polymer processing

The soil release factor for polymer processing has been set at value of 0.1% based on information supplied in Table A3.11 of the EU Technical Guidance Document on Risk Assessment (EC, 2003). The listed value was taken from the polymer industry category (IC-11) and applies to the processing of thermoplastic resins. Further, the most appropriate chemical class was determined to be processing aids rather than solvents since it provides a more representative and conservative determination of the release that may accompany the processing of thermoplastic polymers. Since the soil release factors listed in the A-Table for other types polymer additives are all less than 0.1%, the recommended value is suitably conservative and can be used with all types of volatile materials used in polymer processing.

C. Use in mining

The reagents used for solvent extraction at a mining site can be partly recovered from the crud and reused before disposal of the waste solids. A soil release factor was established using estimates of reagent losses arising from its adsorption onto the crud formed during the extraction process. This crud is formed at the aqueous/organic interface and typically contains a large percentage of organic reagent that may or may not be recovered depending on the economic incentives. An evaluation of organic reagent losses during solvent extraction reported that 50% of the solvent/diluent loss occurs due to entrainment, 25% due to evaporation, and 25% via crud partitioning (Ritcey, 2006). Based on this distribution ratio, the soil release factor of 5% is considered adequate and consistent with the air release factor of 4% established independently.

D. Use as a fuel

Derivation of a soil release factor for the industrial storage and use of fuels is complicated by a lack of reliable information on fugitive spill and leak volumes in and around the bulk fuel tanks serving an industrial gas turbine. Some reasonable and well-vetted surrogate information is available from Concawe-sponsored surveys of European oil pipeline leaks (Concawe, 2021). A recently published multi-year summary provides soil spill volumes that have been normalized according to the throughput of oil in the pipeline. The spills described in the report take into consideration losses resulting from the storage and transfer of oil as well as mechanical failures at pump stations, operational repair problems, and corrosion issues. A listing of the annual normalized spill volumes from 1971 to 2019 shows that the spill volumes did not exceed 10 parts per million parts of oil transported in the pipeline. This value is equivalent to a soil release factor of 0.001% after applying a part-per-million to part-per-hundred conversion factor of 10,000. This recommended factor provides a good worst-case approximation of the soil release factor for the large-scale use of fuels at a power plant with an accompanying auxiliary tank farm.

Table 9. SpERC release factors for soil

Assignments	**SpERC title**			
	water treatment	**polymer processing**	**mining chemical use**	**fuel use**
ERC	3	4	4	7
Soil release factor (%)	0	0.01	5.0	0.001
Source	professional judgement	(EC, 2003)	(Ritcey, 2006)	(Concawe, 2021)

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 product formulators and users to conserve resources, optimize operations, and implement new sustainability initiatives that promote alternative applications for these residues and by-products (EEA, 2016).

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

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

An LCA for polymer manufacturing provided a solid foundation for determining an appropriate waste factor for the polymer processing SpERC (Plastics, 2005). The assessment examined the production of high-density polyethylene from olefin monomers. The amount of incinerated solid waste generated during polymer production was stated to 870 mg/kg

(0.09%). This value was rounded upward to 0.1% to ensure an adequate depiction of this life cycle stage. An uncertainty factor of has not been applied to this value because the quantity of hazardous waste is not expected to appreciably vary for other polymer processing operations.

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

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

Table 10. SpERC waste release factors and their literature source

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

6. Wastewater Scaling Principles

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

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

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

Where:

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

Equation 4 shows that a proportionality relationship exists between the use conditions associated with a SPERC and the use conditions that actually exist at a DU site (ECHA, 2008). This relationship forms the basis for ensuring conformity when the wastewater operating conditions differ at a DU site. The scalable parameters described in equation 4 are not equally applicable to every type of environmental risk. As depicted in equations 5-7, the number of scalable parameters increases as the environmental risk of concern become more removed from the wastewater treatment site (CEFIC, 2012). Consequently, the environmental risk to (1) STP microorganisms, (2) organisms residing in the water column and sediment (i.e., freshwater and marine plants and animals), and (3) apical freshwater and marine predators in the aquatic food chain (i.e., secondary poisoning) utilize slightly different scaling equations. Environmental risk is adequately controlled at each trophic level if the following relationships are maintained and the calculations from the SpERC side of the equations are greater than or equal to the results obtained using the site-specific parameters.

Scaling for environmental risk to wastewater treatment plant microorganisms:

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

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

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

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

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

The total removal efficiency (RE_{total}) is equal to the product of the removal efficiencies attained using onsite and offsite abatement technologies and is calculated as shown in equation 8.

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

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

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

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

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

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

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

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

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

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