<table>
<tr><th>FS Section</th><th>Content field</th><th>Explanation of content</th><th>CSR[1]</th><th>eSDS[2]</th></tr>
<tr><td rowspan="2">1. Title</td><td>1.1 Title of SPERC.</td><td>IFRA - Formulation of fragrance compound</td><td>Y</td><td>Y</td></tr>
<tr><td>1.2 SPERC code:</td><td>IFRA 2.1a.v1 : IFRA - Formulation of fragrance compounds at large/medium sites

IFRA 2.1b.v1: IFRA - Formulation of fragrance compounds at small</td><td>Y</td><td>Y</td></tr>
<tr><td rowspan="2">2. Scope</td><td colspan="4">2.1 Substance/Product Domain</td></tr>
<tr><td>Substance types / functions / properties included or excluded:</td><td>Usually, fragrance ingredients are formulated twice:
- several ingredients are mixed together to make a fragrance compound: this is referred to as the “compounding” stage;
- a fragrance compound is mixed with other ingredients to make a consumer product (e.g. a shampoo): this is referred to as the “formulation” stage.

The scope of this fact sheet covers only the compounding stage. Formulation of fragranced end-products is covered by AISE and COLIPA spERCs Factsheets (http://www.aise.eu/reach/?page=exposureass_sub4 and http://www.cosmeticseurope.eu/safety-and-science-cosmetics-europe/reach-and-chemicals/use-and-exposure-information.html).

Substance Domain: Applicable to individual fragrance substances, stabilizers and solvents that may also be added to enhance the function of the compound, used continuously during all days of the year. The final concentration of a fragrance substance in the fragrance compound can range from parts per million by mass up to 20% w/w. On average a fragrance compound contains 40-60 different fragrance substances.

Size of compounding sites: compounding sites have been assigned to three relative sizes of operations, large, medium and small, based on quantity of fragrance compound produced per year on one compounding site (described below).

Size of compounding sites
Large and medium compounding sites have been aggregated in a single spERC as no major differences in operating conditions and environmental release were observed in an industry survey (Haskoning 2008).

<table>
<tr><th>Size of compounding sites</th><th>Quantity of fragrance compound produced per year on one site (t/y)</th></tr>
<tr><td>Small</td><td>< 1,000</td></tr>
<tr><td>Medium</td><td>1,000 - 10,000</td></tr>
<tr><td>Large</td><td>> 10,000</td></tr>
</table>

Operations covered: Mixing of individual fragrance substances with other fragrance substances, stabilizers and solvents to create a mixture (named fragrance compound), including reception of goods, packing and re-packing of the substance and its mixtures in batch or continuous</td><td>Y</td><td>N</td></tr>
</table>

[1] Explanations that are more detailed can be provided for the CSR..

[2] For the ES for communication a standard phrase may be selected from the ESCom catalogue when available. When no phrase is available yet in the catalogue the proposed phrase can be reported here.

FS Section	Content field	Explanation of content	CSR[1]	eSDS[2]
		operations, including storage, materials transfers, filling process equipment, mixing of ingredients, filling of containers, large and small scale packing, sampling, cleaning, maintenance and associated laboratory activities.		
	Additional specification of product types covered:	n/a	Y	N
	Inclusion of sub-SPERCs: y/n	IFRA 2.1a.v1 : IFRA - Formulation of fragrance compounds at large/medium sites IFRA 2.1b.v1: IFRA - Formulation of fragrance compounds at small	N	N
	2.2 Process domain			
	Description of activities/processes: freetext	Individual fragrance substances are mixed with other fragrance substances to create a mixture (fragrance compound). Dosing, mixing and filling may be a completely automated process for larger batches whereas the small batches may be processed automatically (e.g. via robot) or manually.	Y	N
	2.3 List of applicable Use Descriptors			
	LCS: picklist (select one)*	Formulation or re-packing	Y	Y
	SU: picklist (multi-select)*	SU3 – Industrial uses SU10 - Formulation	Y	Y
	PC: picklist (multi-select)*	No product category	Y	Y
3. Operational conditions	**3.1 Conditions of use**			
	Location of use: pick-list*	Indoor	Y	Y
	Water contact during use: y/n	yes	Y	Y
	Connected to a standard municipal biological STP: y/n	The wastewater is consistently discharged to a biological treatment plant (activated sludge) which is either on the site or a municipal sewage treatment plant.	Y	Y
	Rigorously contained system with minimisation of release to the environment: y/n	No	Y	N
	Further operational conditions impacting on releases to the environment. Free-text **	**IFRA 2.1a.v1: spERC specific Operational Conditions** - The number and sizes of batches is variable (surveyed sites reported from 13 up to 140 batches per day). Naturally, small number of batches is produced in larger quantities; - Dosing is a mixture of automatic and manual dosing. **IFRA 2.1b.v1: spERC specific Operational Conditions** - The number and sizes of batches is variable (surveyed sites reported from <1 up to 15 batches per day). Naturally, small number of batches is produced in larger quantities; - Dosing is mainly a manual process.	Y	Y

FS Section	Content field	Explanation of content	CSR[1]	eSDS[2]
		Operational Conditions common to both spERCs - Compounding is carried out as a batch-wise process; - After each batch a number of mixing vessels will need to be cleaned; - The delivery area is a contained area so spills and contaminated rain is drained to the water treatment system; - Generally the empty containers are not cleaned but they are either dedicated containers or they are recycled by an external company; - Pumps may be cleaned with water and the water is discharged into the drains. Some minor losses may occur there. Estimated losses range from <<0.01% to 0.08%; - Mixing vessels and batch sizes span a large volume range, from a few litres to many cubic meters; - The main release occurs after the mixing process when containers, pumps and other equipment are cleaned with water, detergent and sometimes steam or alcohol. The average releases range from 0.015 to 0.1%, with higher estimates for small batches (< 60L) up to 0.3%. These results are based on measurements; - During the filling of all finished products, rinsing or cleaning procedures are directed towards avoiding emissions to wastewater. Estimated emissions are in the range of 0.01%; • Floors are mopped and the water is discharged to the sewer system; spills are absorbed and treated as chemical waste, although small spills may be washed down the drain.		
	3.2 Waste Handling and Disposal			
	Waste Handling and Disposal: Picklist (multi-select) **	Waste is treated under national regulations. Spills are absorbed and collected as chemical waste. The same is true for samples, packaging materials and sludge residues from water treatment. It is disposed of to an outside contractor and may be treated, incinerated on put in a landfill, according to local regulations. The wastewater is consistently discharged to a biological treatment plant (activated sludge) which is either on the site or a municipal sewage treatment plant. **Picklist (not exhaustive):** • **No (low risk);**	Y	Y
4a. Obligatory RMMs onsite	**RMM limiting release to air:** freetext **	No RMMs needed.	Y	Y
	RMM Efficiency (air): numerical value	/	Y	Y
	Reference for RMM Efficiency (air): freetext	/	Y	N
	RMM limiting release to water: freetext **	/	Y	Y
	RMM Efficiency (water): numerical value	/	Y	Y
	Reference for RMM Efficiency (water): freetext	/	Y	N
	RMM limiting release to soil: freetext **	/	Y	Y
	RMM Efficiency (soil): numerical value	/	Y	Y
	Reference for RMM Efficiency (soil): freetext	/	Y	N
	On-site physico-chemical treatment (before discharging into either a	- It is common practice that the waste water is treated in a physical-chemical system before it is discharged into a biological wastewater		

FS Section	Content field	Explanation of content	CSR[1]	eSDS[2]
4b. Optional RMMs onsite	biological wastewater treatment plant on-site or in a municipal sewage treatment plant)	treatment plant on-site or in a municipal sewage treatment plant.[3] The efficiency of this treatment depends on substance properties such as log Kow and should be considered with care. More especially the validity of this RMM is to be challenged for hydrophilic substances in oil/water separators. The survey of 7 operating plants reported removal efficiencies from 30 to 70%. Individual plants may vary and data collection will be needed to verify a particular treatment plant efficiency.		
	On-site biological treatment (before discharging into a municipal sewage treatment plant)	A biological treatment plants is often present on the larger industrial sites[6]. The efficiency of this RMM varies depending on the treatment technology and the properties of the substance as log Kow and the biodegradability. SimpleTreat is a conservative approach to estimate removal efficiency from biological treatment.		
5. Exposure Assessment Input	**5.1 Substance use rate**			
	Amount of substance use per day: numerical value	No accurate substance maximum use rate in a typical operation can be determined	Y	Y
	Fraction of EU tonnage used in region:	**IFRA 2.1a.v1 spERC**: 1 **IFRA 2.1b.v1 spERC**: 1	Y	N
	Fraction of Regional tonnage used locally:	**IFRA 2.1a.v1 spERC**: 0.25 Based on compounding site survey, the largest user uses a maximum of 25% of the total use volumes (9S3975.01/R0002/Nijm, 2009, cited in IFRA guidance). **IFRA 2.1b.v1 spERC**: 0.02 Based on compounding site survey, small size compounding companies use circa 10% of the total use volume(9S3975.01/R0002/Nijm, 2009, cited in IFRA guidance).. A value of 20% is taken as worst case for the EU tonnage for use of formulation of fragrance compounds by small sites. There are numerous small sites widely dispersed through Europe. A regional percentage of 10% of the EU tonnage can be considered. The overall regional percentage is therefore 2%.	Y	N
	Justification / information source:	See justification above in "Fraction of EU tonnage used in region"	Y	N
	5.2 Days emitting			
	Number of emission days per year:	250 days/year	Y	Y
	Justification / information source:	Equivalent to number of working days, based on 2002/2003 data and 2008 inquiry to compounders	Y	N
	5.3 Release factors			
	sub-SPERC identifier: IFRA 2.1a.v1	IFRA 2.1a.v1 : IFRA - Formulation of fragrance compounds at large/medium sites	Y	N
	ERC: picklist (select one)*	ERC 2		
	sub-SPERC applicability:	*Size of compounding sites*: compounding sites have been assigned to three relative sizes of operations, large, medium and small, based on quantity of fragrance compound produced per year on one compounding site (described below). **Size of compounding sites** — **Quantity of fragrance compound produced per year on one site (t/y)** Medium — 1,000 - 10,000	Y	N

[3] ibid.

FS Section	Content field	Explanation of content	CSR[1]	eSDS[2]
		Large > 10,000		
		Large and medium compounding sites have been aggregated in a single spERC as no major differences in operating conditions and environmental release were observed in an industry survey (Haskoning 2008).		
	5.3.1 Release Factor – air			
	Numeric value / percent of input amount (Air):	0.025	Y	Y
	Justification of RFs (Air):	Default conservative value from ERC2 Not enough specific data have been collected to derive a specific release factor for compounding sites, even though it is obvious that the default release factor of 2.5% overestimates the emission to air. Indeed, most fragrance substances present a moderate to low volatility, most of substances VP being < 500 Pa (see Table 4 below) while the default release factor of 2.5% is based on highly volatile substances (>1000 Pa). Table 4: analysis of vapour pressure of 998 chemicals used in fragrance products	Y	N

Table 4: analysis of vapour pressure of 998 chemicals used in fragrance products

n =	998	chemicals
>1000 Pa	25	chemicals
<1000 Pa	973	chemicals
min =	8.20E-05	Pa
max =	9.999E+04	Pa
median =	2.8	Pa
99-percentile =	3258	Pa
97.5-percentile =	999	Pa
95-percentile =	453	Pa
90-percentile =	156	Pa

FS Section	Content field	Explanation of content	CSR	eSDS
	5.3.2 Release Factor – water			
	Numeric value / percent of input amount (Water):	0.002	Y	Y
	Justification of RFs (Water):	A survey was conducted in 2008 to obtain information on the emission to water during the compounding process[4]. Responses to the questionnaire were received from 7 compounding sites with varying size and varying degree of emission control. Most responses showed that the COD in wastewater was caused mainly by the presence of fragrances in the water. Based on indications of the COD and the production volumes, and assuming that the COD of most of the fragrance ingredients in wastewater = 3 mg O/mg substance it was possible to estimate the release of products to wastewater.	Y	N

[4] ibid.

		This fraction, prior to any treatment, ranges from 0.2 to < 0.43 % for the small compounders whereas for the large compounders the estimates range from 0.01 to 0.15%.		
	5.3.3 Release Factor – soil			
	Numeric value / percent of input amount (Soil):	0	Y	Y
	Justification of RFs (Soil):	All solid waste is collected. Used packaging which has been in contact with chemicals are recycled, collected by waste companies or incinerated. The delivery area as well as the mixing halls is in contained area, so all water is collected in dedicated sewers. This implies that there is no direct emission to the soil. Spills are cleaned with specific sorbing materials or cleaned with water that is collected in dedicated sewers along with the process water. Spilled fragrances may be collected and recycled in the process.	Y	N
	5.3.4 Release Factor – waste			
	Percent of input amount disposed as waste:	0	Y	N
	Justification of RFs:	All solid waste is collected. Used packaging which has been in contact with chemicals are recycled, collected by waste companies or incinerated. The delivery area as well as the mixing halls is in contained area, so all water is collected in dedicated sewers. This implies that there is no direct emission to the soil. Spills are cleaned with specific sorbing materials or cleaned with water that is collected in dedicated sewers along with the process water.	Y	N
	sub-SPERC identifier: IFRA 2.1b.v1	IFRA 2.1b.v1: IFRA - Formulation of fragrance compounds at small	Y	N
	ERC: picklist (select one)*	ERC 2		
	sub-SPERC applicability:	*Size of compounding sites*: compounding sites have been assigned to three relative sizes of operations, large, medium and small, based on quantity of fragrance compound produced per year on one compounding site (described below). **Size of compounding sites** — **Quantity of fragrance compound produced per year on one site (t/y)** Small — <1,000	Y	N
	5.3.1 Release Factor – air			
	Numeric value / percent of input amount (Air):	0.025	Y	Y
	Justification of RFs (Air):	Default conservative value from ERC2 Not enough specific data have been collected to derive a specific release factor for compounding sites, even though it is obvious that the default release factor of 2.5% overestimates the emission to air. Indeed, most fragrance substances present a moderate to low volatility, most of substances VP being < 500 Pa (see Table 4 below) while the default release factor of 2.5% is based on highly volatile substances (>1000 Pa). Table 4: analysis of vapour pressure of 998 chemicals used in fragrance products n = — 998 — chemicals >1000 Pa — 25 — chemicals	Y	N

		<1000 Pa | 973 | chemicals min = | 8.20E-05 | Pa max = | 9.999E+04 | Pa median = | 2.8 | Pa 99-percentile = | 3258 | Pa 97.5-percentile = | 999 | Pa 95-percentile = | 453 | Pa 90-percentile = | 156 | Pa		
	5.3.2 Release Factor – water			
	Numeric value / percent of input amount (Water): numerical value	0.005	Y	Y
	Justification of RFs (Water): freetext	A survey was conducted in 2008 to obtain information on the emission to water during the compounding process[5]. Responses to the questionnaire were received from 7 compounding sites with varying size and varying degree of emission control. Most responses showed that the COD in wastewater was caused mainly by the presence of fragrances in the water. Based on indications of the COD and the production volumes, and assuming that the COD of most of the fragrance ingredients in wastewater = 3 mg O/mg substance it was possible to estimate the release of products to wastewater. This fraction, prior to any treatment, ranges from 0.2 to < 0.43 % for the small compounders whereas for the large compounders the estimates range from 0.01 to 0.15%.	Y	N
	5.3.3 Release Factor – soil			
	Numeric value / percent of input amount (Soil):	0	Y	Y
	Justification of RFs (Soil):	All solid waste is collected. Used packaging which has been in contact with chemicals are recycled, collected by waste companies or incinerated. The delivery area as well as the mixing halls is in contained area, so all water is collected in dedicated sewers. This implies that there is no direct emission to the soil. Spills are cleaned with specific sorbing materials or cleaned with water that is collected in dedicated sewers along with the process water. Spilled fragrances may be collected and recycled in the process.	Y	N
	5.3.4 Release Factor – waste			
	Percent of input amount disposed as waste:	0	Y	N
	Justification of RFs:	All solid waste is collected. Used packaging which has been in contact with chemicals are recycled, collected by waste companies or incinerated. The delivery area as well as the mixing halls is in contained area, so all water is collected in dedicated sewers. This implies that there is no direct emission to the soil. Spills are cleaned with specific sorbing materials or cleaned with water that is collected in dedicated sewers along with the process water.	Y	N
References to SPERC Background Document [6]				

[5] ibid.

[6] The objective of this factsheet is to summarize the SPERC key facts provided in the corresponding SPERC background documents. It gives an overview of the SPERC essentials for the chemical safety assessment. A SPERC background document is a reference document, which provides the description of the emission situation(s) for a use specified by an industrial sector, the justification and applicability domain of the environmental release factors, and the references/information sources/methods used in the derivation of the release factors.

	Reference to Background Document	Review and evaluation of environmental emission scenarios for fragrance materials during compounding of perfume oils and formulation of consumer products (RIFM, 2009, https://www.rifm.org/publications-detail.php?id=77#gsc.tab=0)	Y	N

* picklists with exhaustive lists of phrases are available as ESCom phrases
** the content may be adopted from ESCom phrases