

Phenol & Derivatives – REACH Consortium

Qualitative Environmental Exposure Assessment

ACETONE

CAS No: 67-64-1

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Table of Content

1. ENVIRONMENTAL EXPOSURE	3
1.1 General discussion	3
1.2 Production	3
1.3 Uses	4
1.4 Natural and further releases into the environment	4
2. ENVIRONMENTAL DISTRIBUTION AND BEHAVIOUR	6
2.1 Distribution	6
2.2 Degradation	7
2.3 Bioaccumulation	7
3. BACKGROUND LEVELS	7
4. ECOTOXICOLOGICAL INFORMATION	8
4.1 Aquatic environment	8
4.2 Terrestrial environment	8
5. CLASSIFICATION FOR THE ENVIRONMENT	8
6. REFERENCES	10
APPENDIX I	13

1. Environmental Exposure

1.1 General discussion

Acetone is released from a number of both human-made as well as natural sources. Man-made releases are quite small compared to natural sources of acetone in the environment. Releases to the environment by producers, processors and users of acetone have been estimated to represent only about 1-2 percent of total annual environmental loading. Approximately 97 percent of annual environmental loading come from natural sources (vegetative releases, forest fires and other natural sources) and the photo-oxidation of alkanes and alkenes (OECD 1999, VCCEP 2003).

The purpose of this chapter is to reflect qualitatively the exposure situation in the EU that results from industrial sources of acetone production and processing. As far as exposure of the environment is concerned, the diffuse emissions of acetone from natural sources by far exceed the industrial emissions.

In the appendix predefined environmental exposure scenarios are attached to this document. These enable downstream users of acetone to check and reflect their specific exposure situation in regard to surface-water and soil release and to determine their conditions for a safe use as well as their acceptable use volumes. Reference is given to an according tool, that is enclosed in the registration dossier as an attached document (ECT_Acetone_19Jul2010.xls) and may be downloaded from the P&D REACH Consortium-website or the web-site of the consortium members.

1.2 Production

Worldwide production capacity of acetone was 3.8 million tonnes in 1995 with the actual volume produced being somewhat less at 3.7 million tonnes. Production capacity in the United States constituted about 33% (1.3 million tonnes) of the global capacity, while the capacity in Western Europe and Asia (including Japan) was about 31% (1.2 million tonnes) and 19% (0.7 Mio tonnes), respectively. For 2008, the CMAI Capacity Database reports a total supply of approx. 5 Mio tonnes worldwide and 1.5 Mio in Western Europe (CMAI, 2010).

Acetone can be manufactured by several routes: (a) as a co-product of phenol via cumene peroxidation, (b) via dehydrogenation of isopropyl alcohol, (c) as a byproduct of hydroquinone production, and (d) as a byproduct of propylene oxide production. The predominant route to production of acetone is the cumene peroxidation process. In this process, benzene is alkylated to cumene which is oxidized to cumene hydroperoxide, which in turn is cleaved to phenol and acetone. Distillation columns are employed to attain desired purity, which is typically greater than 99% for the final product. The processes and equipment for manufacture, transfer and storage are all continuous and enclosed. Equipment and tanks are customarily vented to water scrubbers or through conservation vents to prevent atmospheric loss via evaporation. These practices keep environmental acetone losses during production to a minimum (VCCEP 2003).

The release of acetone by chemical manufacturers' and end users accounts for a very small percentage (1%) of the estimated 40 million tonnes that are annually released to the environment (OECD 1999).

1.3 Uses

Acetone is one of the most widely used industrial solvents. Acetone is used in surface coatings, cleaning fluids, pharmaceutical and cosmetic applications, adhesives and numerous other consumer and commercial products. It also is sold in small containers (e.g., one liter) via various sales channels. Acetone is used in the extraction of fats, oils, waxes and resins from natural products, as a denaturant for ethyl alcohol, and as acetylene absorbent. Acetone is used in the manufacture of cellulose acetate fibers. Acetone also is widely used as a chemical intermediate. Numerous chemicals are produced starting with the self-condensation of acetone to diacetone alcohol, including methyl isobutyl ketone, methyl isobutyl carbinol, hexylene glycol, and isophorone. For 2008, the CMAI Capacity Database (CMAI, 2010) allocates the total supply of acetone to the main industrial sectors of use as follows:

Demand	World	Western Europe
	[approx. percent of supply]	
Bisphenol A	22	18
MMA	23	25
Other chemical derivatives	13	11
Solvents	41	33

1.4 Natural and further releases into the environment

Man-made releases are small compared to natural sources of acetone in the environment. Releases to the environment by producers, processors and users of acetone have been estimated to represent only about 1-2 percent of total annual environmental loading. Approximately 97 percent of annual environmental loading comes from natural sources (vegetative releases, forest fires and other natural sources) and the photo-oxidation of alkanes and alkenes. The remainder comes from anthropogenic biomass burning (VCCEP 2003). According to OECD (1999) the release of acetone by chemical manufacturers' and end users accounts for a very small percentage (1%) of the estimated 40 million tonnes that are annually released to the environment.

Atmosphere

Vegetative releases

Acetone was found to be a product of metabolism in microorganisms, plants and animals. The compound is formed during fermentation by *Clostridiaceae*. In animals, acetone is formed together with acetyl acetic acid and β -hydroxybutyric acid, predominantly during fatty acid metabolism. The compound was measured in human fluids in concentrations of 0.31 – 3.03 mg/L in urine, 0.93 mg/L in blood, 2.9 mg/L in serum, and 0.41 – 4.35 mg/L in plasma (BUA 1996).

Acetone can be found as an ingredient in a variety of consumer products ranging from cosmetics to processed and unprocessed foods. The compound is present in beverages, baked goods, deserts, and preserves at concentrations ranging from 5 to 8 mg/L. It can also be detected in measurable amounts in onions, grapes, cauliflower, tomatoes, milk, cheese, beans, peas, and other natural foods. Milk from dairy cattle may contain very high levels of acetone, ranging as high as 225 mg/L for the milk from hyperketo-nemic cows. Acetone has also been identified, but not quantified, in air samples from numerous plants and microorganisms. In

addition to its elimination in the expired air of all mammals, acetone is excreted as a metabolic end-product by some bacteria (*Clostridium butylicium*), molds, fungi (*Paecilomyces variotii*), and algae (*Cryptomonas ovate palustris*) (OECD 1999).

Vegetative releases, forest fires, and other natural events account for nearly half (47%) of the estimated annual emissions of acetone. The global release by vegetation was estimated to 4 – 18 Mio. t/a (average 9 Mio t/a) (OECD 1999). No release amounts for microorganisms or animals could be identified. Releases into the environment within the EU were not located in the literature.

A rough estimation of European releases can be performed taken into account the continental and the global land area. The global land area is 148,9 Mio. km², while the area of the European Union is 4.3 Mio. km² (Wikipedia 2010), i.e. 2.9% of global. Assuming that the acetone emission by vegetation is equally distributed over the earth, 261,000 t acetone/a (2.9% · 9 Mio. t/a) would be released from vegetative sources in Europe.

Biomass burning

Acetone is often detected as an end product of thermal combustion and biological decomposition. Emissions from poultry manure (530 g/kg), backyard waste incinerators (4.0 g/kg), pine wood combustion (2.8 g/kg), neoprene combustion (990 mg/kg), and wood burning stoves (145 mg/kg) have all been measured and reported (OECD 1999).

The global release by biomass burning was estimated to 8 – 12 Mio. t/a (average 10 Mio t/a) (OECD 1999). Releases into the environment within the EU were not located in the literature.

A rough estimation of European releases can be performed taken into account the continental and the global land area (see above). Assuming that the acetone emission by biomass burning is equally distributed over the earth, 290,000 t acetone/a (2.9% · 10 Mio. t/a) would be released in Europe from biomass burning.

Photooxidation of alkanes and alkenes

Acetone is formed by photo-oxidation of alkanes, e.g. from vehicle exhaust (BUA 1996).

About 50% of the total emissions result from the tropospheric photooxidation of propane and other alkanes and alkenes. The following global sources are reported: propane oxidation 15 – 20 Mio. t/a (average 17 Mio t/a), isobutane & isopropane oxidation 1 – 3 Mio. t/a (average 2 Mio t/a), isobutene & isopropene oxidation 1 – 2 Mio. t/a (average 1 Mio t/a), and myrcene oxidation 0.2 – 0.3 Mio. t/a (average 0.2 Mio t/a). The average global release due to these sources is 20.2 Mio t/a (OECD 1999).

The release estimation in OECD (1999) was based on data from the 1990ies. Recent investigations demonstrate that the emissions from vehicle exhaust decreased significantly in the last decade. According to LUBW (2010) benzene concentrations measured at traffic monitoring stations dropped from ca. 10.7 µg/m³ in 1996 to 2.3 µg/m³ in 2008. Similar results were published in UBA (2010): benzene concentrations measured in urban traffic areas decreased from 7.9 µg/m³ in 1997 to 2.1 µg/m³ in 2007, while urban background concentrations decreased from 2.8 µg/m³ to 1.0 µg/m³ in the same period. In the same period industrial hydrocarbon emissions decreased drastically. Therefore, acetone emissions estimated in OECD (1999) could overestimate the current situation. Furthermore, only a part of the global release is emitted within the European Union. For the exposure estimation it is assumed that approximately 10% of the reported amount (= 2.02 Mio. t/a) is released within the EU.

2. Environmental distribution and behaviour

2.1 Distribution

Deduced as a weight of evidence from the physicochemical data (miscibility with water in all proportions, $\log P_{ow} = -0.24$) acetone should not adsorb onto soils. Data for soil sorption are quoted in a reliable scientific study. Soil sorption K_d was 1.5 L/kg, at 20 °C. The soil sorption coefficient indicates that acetone is mobile in soil and may be transported by soil water (Roy W, Griffin R 1990).

Several reliable experimental studies and further reported values for the Henry's Law constant are available. According to reliable experimental studies (bubble column technique) the Henry's Law constant was determined to 2.929 Pa m³mol⁻¹ (Zhou X, Mopper K 1990) and 3.070 Pa m³mol⁻¹ at 25 °C (Betterton E 1991), indicating a moderate volatility from water. The Henry's law constant for sea water was determined to 3.311 Pa m³mol⁻¹ at 25 °C. A slight salting-out effect is to be observed by comparison of the Henry's Law constants in fresh and sea water (Zhou X, Mopper K 1990). In both media the Henry's law constants rise with temperature.

Distribution modelling using a simple one-dimensional model of the global circulation assuming a single pulse emission of acetone predicted significantly high spatial ranges of 46.5% of the earth perimeter, which are caused by their intermediate gas-phase stability and high volatility. The persistence's are predicted below 20 days, mainly due to the degradation in water and soil (Scheringer M 1997).

A generalised (STP) Fate Model based on a steady-state mass balance model designed for primary and biological reactors of a typical diffused air activated sludge system considering the processes advection, sorption, volatilisation, air stripping, and biotransformation was used to predict the fate of acetone in waste water plants. The model calculations implicate that acetone is predominantly in the aqueous phase and without biotransformation it would be transferred to the effluent. Volatilisation is not relevant. In model runs including biodegradation removal is partly due to biotransformation and to transport to the effluent (Byrns G 2001).

There are several studies concerning other distribution data dealing with the partition of acetone between air and water and the behaviour in soils. Air/water partition coefficients range from 357 – 341:1 (Cowan J 1990), these data are in accordance with the moderate volatility of acetone deduced from the experimentally derived Henry's Law constants.

Other studies are dealing with the diffusion of acetone in soil air. Soil diffusion coefficient at 0 °C was calculated for 8.8 x 10⁻³cm²/sec (Roy W, Griffin R 1990). The diffusion coefficient for acetone was found to be considerably lower than in air. Liquid acetone is able to expand clay soils rapidly within 2-3 days to an extent of 3.5 – 8 % (Green W et al. 1983).

The calculated theoretical distribution in the environment (distribution model according to Mackay, level 1) clearly demonstrates that the atmosphere and hydrosphere are the target compartments for acetone in the environment (OECD 1999):

Air:	71.00 %
Water	28.58 %
Soil	0.00 %

Sediment 0.01 %

2.2 Degradation

Acetone introduced in water has been shown to be **readily biodegradable** in a considerable number of reliable investigations under a wide variety of conditions (including anaerobic conditions). This holds also true also for biodegradability in sediment as well as soil. Taking into account the ubiquitous occurrence of acetone in environmental compartments, adaptation is to be assumed in the case of microbial inocula.

There are two reliable experimental studies for photo degradation in air. The overall loss rate of acetone including photo dissociation and loss by reaction with OH radicals and the corresponding lifetimes were calculated for January, Equinox and July at 40 degree northern latitude. Lifetimes were reported to be 18.6 - 114.4 days. This results correspond to the findings of the second study where the photo dissociation lifetime for 40°solar angle is reported to be $1/k_{\text{dissoc}} = 14.8$ days.

2.3 Bioaccumulation

No reliable experimental data on bioaccumulation are available. Based on the calculated BCF=3 (input parameter: measured log Kow value) no potential for bioaccumulation is to be expected (Fh-ITEM 2009).

3. Background levels

Recent monitoring data are not available. Most of the available studies refer to atmospheric concentrations.

Acetone concentrations in remote areas (Pt Barrow, Alaska, USA, 1967) were found to be 0.72 – 6.96 $\mu\text{g}/\text{m}^3$ (Verschueren 1983, Cavanagh, LA et al. 1969). At rural sites in the USA, acetone concentrations were determined for 0.72 – 2.16 $\mu\text{g}/\text{m}^3$ in 1971 (Robinson E et al. 1973). Mean Concentrations at rural sites (Arizona, USA, 1982) were found to be 6.2 $\mu\text{g}/\text{m}^3$ (SD: ± 0.8). Somewhat higher mean concentrations of 28.8 $\mu\text{g}/\text{m}^3$ (SD: ± 4) were found at urban sites (Tucson, Arizona, USA) (Snider JR, Dawson GA 1985). In at urban sites in Sweden (Stockholm, 1982/83) mean concentrations of acetone in air were in the same order of magnitude 9.7 — 46.6 $\mu\text{g}/\text{m}^3$. Possible sources other than vehicle exhaust as solvent use, photochemical oxidation or biogenic sources were discussed. There was no statistically significant correlation with traffic exhaust components as CO and benzene (Jonsson A 1985). Mean ambient air concentrations in Northern Italy in 1983 – 1984 were found to be 39 $\mu\text{g}/\text{m}^3$ (indoor, range: 3 – 157 $\mu\text{g}/\text{m}^3$) and 6 $\mu\text{g}/\text{m}^3$ (outdoor, range: <2 – 16 $\mu\text{g}/\text{m}^3$) (Verschueren 1983).

For fresh water no background concentrations are available.

In the USA some studies were performed at contaminated sites. In a contaminated well 3 $\mu\text{g}/\text{L}$ acetone were determined (Rao PSC 1985). 0.56 – 600 mg/L acetone was measured in landfill leachate (Verschueren 1983). 0.2 — 0.7 $\mu\text{g}/\text{L}$ acetone was found in six drinking water wells in the vicinity of a solid waste landfill. In the landfill leachate 43.700 $\mu\text{g}/\text{L}$ acetone was detected (DeWalle FB, Chian ESK 1981).

In contrast background concentrations in sea water are available. Acetone concentrations were determined for 0.014 — 0.052 mg/L (Straits of Florida) and 0.018 — 0.053 mg/L (Eastern Mediterranean) acetone (Corwin J 1969).

In sludge from the wwtp Bottrop of the Emscher Genossenschaft (receiving the wastewater of INEOS phenol) a concentration of 1.5 mg/l acetone was measured in 2010 (Emscher Genossenschaft, 2010).

2.4 – 44 mg/kg dw acetone was determined in soils (Colorado, USA, 1978) by a purge and trap method. Acetone occurred in all soils tested. The addition of lime increased emission of acetone in the three acid soils tested (Pavlica D et al. 1978).

According to handbook data acetone is a normal micro component in blood and urine, a minor constituent in pyroigneous acid and an oxidation product of alcohols and humic substances (Verschueren 1983). In cigarette smoke 2640 mg/m³ and gasoline exhaust (partly propionaldehyde) 5.52 – 33.6 mg/m³ were determined (Verschueren 1983).

Based on the releases referred in Ch. 1.4, the following regional environmental concentrations were estimated by EUSES 2.1.1:

PEC_{regional}_{aquatic} = 2.29 µg/l

PEC_{regional}_{marine} = 0.759 µg/l

PEC_{regional}_{air} = 12.8 µg/m³

PEC_{regional}_{agr.soil} = 1.9 µg/kg wwt

PEC_{regional}_{natural soil} = 3.69 µg/kg wwt

4. Ecotoxicological information

4.1 Aquatic environment

Short-term toxicity data for fish (freshwater), invertebrates (freshwater and marine water), and algae (freshwater and marine water) as well as long-term toxicity data for freshwater invertebrates and algae are available. Algae proved to be the most sensitive fresh water organism (*Mycrocystis aeruginosa*: 8 d TT (NOEC)=530 mg/L nominal). Based on the available reliable results (results of acute toxicity testing from three trophic levels and long-term toxicity testing from two trophic levels) an assessment factor of 50 seems to be justified according to TGD. Based on this, the **PNEC aqua (freshwater)=10.6 mg/L** is obtained.

4.2 Terrestrial environment

There are no data available from guideline studies using sediment as test medium. In the absence of ecotoxicological data for sediment-dwelling organisms, the PNEC_{sed} may be provisionally calculated using the equilibrium partitioning method according to ‘Guidance on information requirements and chemical safety assessment Chapter R.10 –Dose [concentration]-response regarding environment’ (ECHA 2008). With the default parameters of the TGD concerning the fractions and densities in sediment as well as the substance parameters, the calculation of **PNEC soil resulted in a value of 23.9 mg/kg wet soil**.

5. Classification for the environment

Due to its **ready biodegradability** in the environment as well as its insignificant potential for bioaccumulation, acetone is not classified as dangerous/hazardous for the environment according to Directive 67/548/EEC and according to the Regulation (EC) 1272/2008 on classification, labelling and packaging of substances and mixtures (CLP Regulation):

According to Directive 67/548/EEC Annex 1 (environment): not classified

According to CLP - (EC) 1272/2008 (environment): not classified

L(E)C50 >100 mg/L; readily biodegradable, no bioaccumulation

Hazardous to the atmospheric environment:

(Hazardous to the ozone layer: This includes substances which are listed in Annex I to Regulation (EC) No 2037/2000 of the European Parliament and of the Council on substances that deplete the ozone layer (1) and its subsequent amendments):

Acetone is not listed in Annex I of (EC) No 2037/2000.

M-Factor: No

Labelling No Signal word and Pictogram for environmental hazards

6. References

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Appendix I

Predefined Emission Scenarios

Predefined emission scenarios Sheets are presented for acceptable environmental emissions in soil and surface water (PECsoil and PECsurface water).

The sheets contain maximum acceptable use volumes dependent on the local situation (e.g. ERC, dilution).

An according ECT-tool can be downloaded from the P&D REACH-Consortium web-page or the web-site of the producers. It is based on EUSES but with some simplifications to improve the user friendliness and to concentrate on the key-parameters

Predefined emission scenarios for Acetone (PECwater)

Use volume (t/a)	Local Release factor (%)	Removal rate (%)	dilution factor (-)	Acceptable volume (t/a)	Defined for ERC	suitable also for ERC
Default		88	10			
Site specific		88 .. 98.5	20 ... 160			
<641	100	88	10	641	4 8a 8d 10 b 11b	all
<1000	100	88	20	1283	4 8a 8d 10 b 11b	all
<1000	100	93	10	1100	4 8a 8d 10 b 11b	all
<1000	100	93	100 (sea release)	1100	4 8a 8d 10 b 11b	all
<5000	100	88	80	5134	4 8a 8d 10 b 11b	all
<5000	50	88	40	5134	5	all except 4 8a 8d 10 11b
<5000	50	97	100 (sea release)	5134	5	all except 4 8a 8d 10 11b
<10000	50	88	80	10268	5	all except 4 8a 8d 10 11b
<10000	50	95,5	30	10268	5	all except 4 8a 8d 10 11b
<10000	6	88	100 (sea release)	10696	1	all except 4 5 8a 8d 10b 11b
<10000	6	88	10	10696	1	all except 4 5 8a 8d 10b 11b
<50000	6	88	50	53482	1	all except 4 5 8a 8d 10b 11b
<50000	6	97,5	100 (sea release)	51343	1	all except 4 5 8a 8d 10b 11b
<50000	6	94	25	53482	1	all except 4 5 8a 8d 10b 11b
<50000	2	88	25	64197	2 6a 8b 8e	3 6d 8c 8f 10a 11a
<100000	6	88	100	106965	1	all except 4 5 8a 8d 10b 11b

<100000	2	96,5	100 (sea release)	110021	2 6a 8b 8e	3 6d 8c 8f 10a 11a
<100000	1	92,5	100 (sea release)	102686	8c 8f	3 6d 10a 11a
<100000	1	88	20	128358	8c 8f	3 6d 10a 11a
<500000	2	88	160	513433	2 6a 8b 8e	3 6d 10a 11a
<500000	1	98,5	100 (sea release)	513433	8c 8f	3 6d 10a 11a
<500000	1	88	80	513433	8c 8f	3 6d 10a 11a
<500000	0,2	93	100 (sea release)	550107	3	6d 10a 11a

Predefined Environmental Release Classes

ERC	Environmental Release Class	Default Release Fraction
ERC 1	Production of chemicals	6,00%
ERC 2	Formulation of preparations	2,00%
ERC 3	Formulation in articles	0,20%
ERC 4	Industrial use of processing aids	100,00%
ERC 5	Industrial use resulting in inclusion into or onto a matrix	50,00%
ERC 6a	Industrial use of intermediates	2,00%
ERC 6b	Industrial use of reactive processing aids	5,00%
ERC 6c	Production of plastics	5,00%
ERC 6d	Production of resins/rubbers	0,005%
ERC 7	Industrial use of substances in closed systems	5,00%
ERC 8a	Wide dispersive indoor use of processing aids in open systems	100,00%
ERC 8b	Wide dispersive indoor use of reactive substances in open systems	2,00%
ERC 8c	Wide dispersive indoor use resulting in inclusion into or onto a matrix	1,00%
ERC 8d	Wide dispersive outdoor use of processing aids in open systems	100,00%
ERC 8e	Wide dispersive outdoor use of reactive substances in open systems	2,00%
ERC 8f	Wide dispersive outdoor use resulting in inclusion into or onto a matrix	1,00%
ERC 9b	Wide dispersive outdoor use of substances in closed systems	5,00%
ERC 10a	Wide dispersive outdoor use of long-life articles and materials with low release	0,16%
ERC 10b	Wide dispersive outdoor use of long-life articles and materials with high or intended release	100,00%
ERC 11a	Wide dispersive indoor use of longlife articles and materials with low release	0,05%
ERC 11b	Wide dispersive indoor use of longlife articles and materials with high or intended release	100,00%

Predefined emission scenarios for Actone (Entry route: Sludge and aerial deposition, PECsoil)

Use volume (t/a)	Local Release factor water (%)	Local Release factor air (%)	Acceptable use volume (t/a)	Defined for ERC	suitable also for ERC
<6500	100	100	6516	4 8a 8d 10 b 11b	all
<100000	6	5	118474	1	2 3 6a 6b 6c 8b 8e 9b 10a 11a
<250000	2	2,5	289603	2	8b 8e 10a 11a
<500000	2	0,1	620577	8b 8e	10a 11a
< 6 Mio	0,16	0,05	6205770	ERC 10a	11a
< 13 Mio	0,05	0,05	13032118	ERC 11a	
any	dry sludge <10000 mg/kg	air release below 300000 t/a	any	all	

Predefined Environmental Release Classes

ERC	Environmental Release Class
ERC 1	Production of chemicals
ERC 2	Formulation of preparations
ERC 3	Formulation in articles
ERC 4	Industrial use of processing aids
ERC 5	Industrial use resulting in inclusion into or onto a matrix
ERC 6a	Industrial use of intermediates
ERC 6b	Industrial use of reactive processing aids
ERC 6c	Production of plastics
ERC 6d	Production of resins/rubbers
ERC 7	Industrial use of substances in closed systems
ERC 8a	Wide dispersive indoor use of processing aids in open systems
ERC 8b	Wide dispersive indoor use of reactive substances in open systems
ERC 8c	Wide dispersive indoor use resulting in inclusion into or onto a matrix
ERC 8d	Wide dispersive outdoor use of processing aids in open systems
ERC 8e	Wide dispersive outdoor use of reactive substances in open systems
ERC 8f	Wide dispersive outdoor use resulting in inclusion into or onto a matrix

ERC 9a	Wide dispersive outdoor use of substances in closed systems
ERC 9b	Wide dispersive outdoor use of substances in closed systems
ERC 10a	Wide dispersive outdoor use of long-life articles and materials with low release
ERC 10b	Wide dispersive outdoor use of long-life articles and materials with high or intended release
ERC 11a	Wide dispersive indoor use of longlife articles and materials with low release
ERC 11b	Wide dispersive indoor use of longlife articles and materials with high or intended release