CHEMICAL SAFETY REPORT

Non-confidential report

Legal Name of applicant(s): BASF Schweiz AG
CH 4002-Basel, Switzerland

Site: BASF-Schweizerhalle

Submitted by: BASF Schweiz AG

Substance Name: bis(2-methoxyethyl) ether
EC Number: 203-924-4
CAS Number: 111-96-6

Use title: Use of diglyme as solvent in the manufacturing process of product by process used in the electronic industry in several applications.

Part 1-8 of the Chemical Safety Report submitted to the Swiss Authorities are not part of the non-confidential report.

DECLARATION:

We, BASF Switzerland AG, request that the information which will be blanked out in the "public version" of the Chemical Safety Report is not disclosed. We hereby declare that, to the best of our knowledge of today the information is not publicly available, and in accordance with due measures of protection that we have implemented, a member of the public should not be able to obtain access to this information without our consent or that of the third party whose commercial interests are at stake.

Signature

Schweizerhalle, den 29.07.2019

Date, Place

Dr. Rolf Kugler

Head of Pilot

Signature

Basel, den 29.07. 2019

Date, Place

Patrick Keller

Head of Product Compliance

9. EXPOSURE ASSESSMENT

9.0.1 Introduction and general notes on exposure scenarios

Diglyme is used as a solvent in the industrial synthesis of other chemical substances. Due to its aprotic and polar properties Diglyme is a unique solvent in chemical synthesis. Due to the absence of reactive functional groups Diglyme behaves inert and is thus superior to any other aprotic, polar solvents. Only uses by workers in industrial settings are relevant. Diglyme is not recommended for use in any consumer products.

Overview of uses and exposure scenarios

Diglyme is used as process solvent at BASF's production site Schweizerhalle in Muttenz, Switzerland. It serves as solvent in the manufacturing step of intermediate [redacted] which after further reaction steps is transformed into final product [redacted] a [redacted] resin used in highly complex electronic display components with very narrow product specifications.

The entire production process is performed automatically in a closed system, with no significant opportunity for exposure of workers or release to the environment. Opportunities for exposure are however given during the following steps that require manual intervention:

a) Diglyme charging: The solvent is transferred from transport drums into the closed system (head tank).
b) The wet intermediate is isolated on a [redacted] filter in a closed environment and the mother liquor containing [redacted]% of diglyme is sucked off via pipeline and sent to a storage tank. The wet cake containing traces of diglyme is washed several times and transferred from the operator manually from the [redacted] filter to trays. The trays are placed from the operator into the vacuum oven for drying. The last solvent traces are absorbed in a scrubber. After drying the product is discharged from the oven into drums using a semi-automated filling line.
c) Sampling: From the washed wet cake a sample is taken in a small bottle and brought to the analytical laboratory. The operator takes the sample from the bottle to a tray and

starts the drying process. After drying of the sample, the lab technician takes the sample and analyses the final product for residual water content and inherent viscosity.

d) Waste handling: Transfer of bulk solvent waste (containing ~[redacted] % diglyme) from closed waste storage tank to
    a) an incineration plant or
    b) railroad tankers for transport to an incineration plant [redacted]
    c) From the liquid waste storage tank, a small sample is taken for analytical investigation prior incineration.

Any other process steps do not require manual handling of diglyme-containing materials by personnel. Since the manufacturing system is completely closed there is no significant opportunity for exposure or release to the environment. Transfer of solvent and/or reaction solution between vessels takes place via fixed piping, i.e. within the closed system and hence does not constitute a separate process step that would need to be evaluated.

Preventative maintenance

The entire equipment is serviced on a regular basis (preventative maintenance) according to maintenance plans (MPs) for every component of the facility that requires regular preventative maintenance. Preventative maintenance does not entail any exposure to diglyme, since it is performed prior to the production campaign on equipment devoid of any process chemicals. Therefore, preventative maintenance ensures proper functioning and pressure tightness of the equipment and a maximum level of containment, safeguarding against exposure to diglyme during its use in the synthesis process.

Prior to start of charging and production, the equipment is subjected to a pressure and integrity test to ensure full leak-tightness of the system. Charging and production must not start without passing the integrity test.

Principal working hygiene: Hands, forearms and face are washed thoroughly after handling chemical products, before eating, smoking and lavatory use and at the end of the working period. Contaminated clothing is immediately removed and washed before re-use.

It should also be noted that Diglyme is a flammable liquid that may release explosive vapours. For this reason, strict safety measures apply (earthing of movable vessels and devices, use of explosion-proof equipment, strict avoidance of spills, careful handling of the solvent). Operators

are advised to maintain a high containment level. These measures significantly contribute to minimisation of operator exposure. Operators receive specific training for this task.

Precautionary measures against electrostatic loading are taken. Earthing is established during the loading operation. The total production area is classified Ex2T3.

The whole occupational exposure scenario for the [redacted] process can be broken down into the following contributing scenarios (including those with no opportunity for exposure, and those with potential for exposure above):

Diglyme Charging

Diglyme is charged from drums into the head tank [redacted].
Diglyme drums are stored in a local warehouse ([redacted]) on site before use. In this warehouse [redacted] drums of Diglyme are prepared before charging (see figure 1). The drums are opened sequentially by the operator. A suction lance with a closed valve and a nitrogen inlet valve are installed at each drum. This step takes place outdoors and the operator wears personal protective Equipment (PPE). In addition, as an engineering control measure, a local exhaust system is in place and the suction lance and the nitrogen valves are stored in a vented booth to reduce the exposure to vapours.

A palette with [redacted] closed drums of diglyme is transferred to the production plant. Within the plant building the suction lance and the nitrogen valve are coupled to the solvent station. The head tank [redacted] is evacuated and Diglyme is sucked from the drums to the head tank [redacted] until the drums are emptied. During the charging of diglyme nitrogen is sucked into the drum. The emptied drums are decoupled from the solvent station and brought back to the warehouse. The suction lance and the nitrogen valve are deinstalled and stored in a vented booth to reduce the exposure to vapours.
The empty diglyme drums are sealed and sent to off-site incineration. During this process step the operator wears personal protective Equipment (PPE). In addition, a local exhaust system is in place as an engineering control measure.

Personal protective equipment consists of

a) respiratory PPE: Full Mask (Jupiter system, 3M) with filter type ABEK P3.
b) Skin PPE: Suitable gloves (KCL Vitoject 890) and protective clothing including safety shoes
c) Eye protection: Face shield from Jupiter system

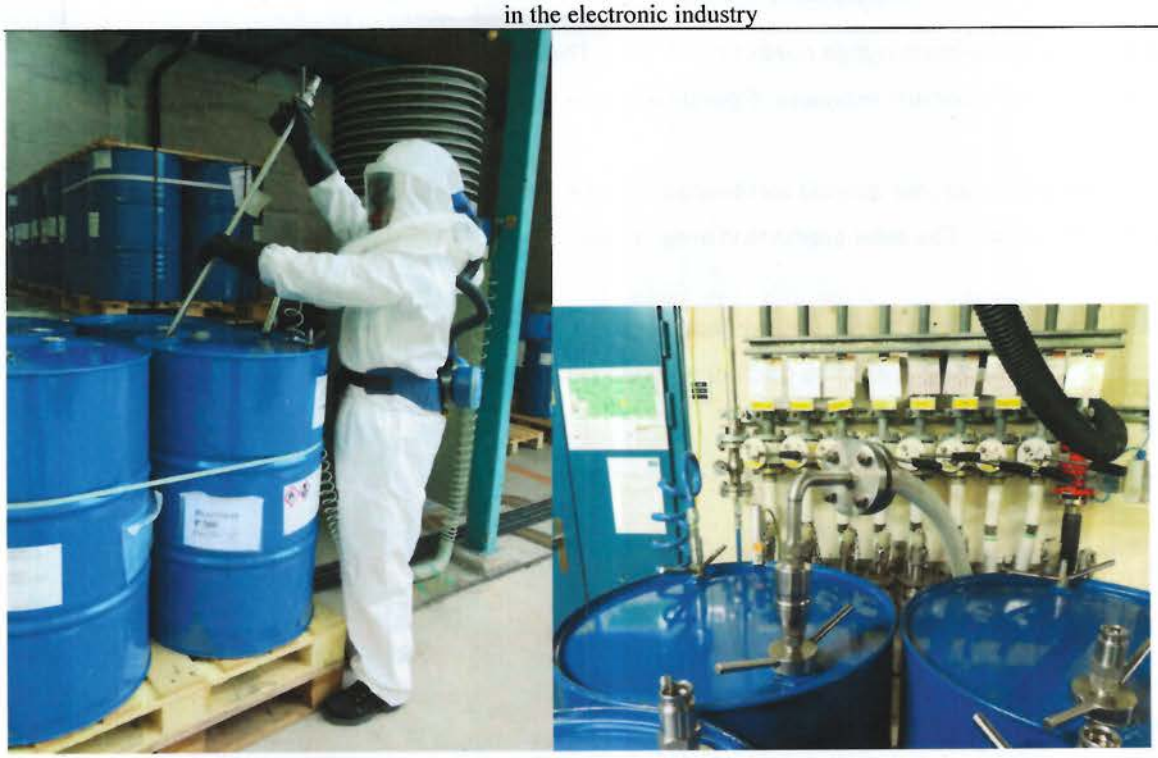

Figure 1: Use of suction lance at the production facility, with connected piping and storage drum

Off-gas treatment and release to the environment: The extract system discharges via water scrubber to atmosphere. However, in view of the small aperture of the drums (max. 7 cm diameter) and the low volume of solvent handled (in total [redacted] L per event) any losses to the atmosphere is expected to be minimal. In the production plant all local ventilation systems are also discharging via water scrubber to atmosphere. There is only a very low diffuse emission of diglyme traces into the air. For the exposure assessment, the release to air has been taken into account using the very conservative default values from ERC 7 (5% release to air) which is definitely a worst-case assumption.

Reaction phase (synthesis in a closed system)

This process is fully automated, taking place in a completely closed reactor system. Planned maintenance is scheduled once per year (see preventative maintenance). Manual interference is not required. The process is supervised by remote control from a control room. Process synthesis tasks for operators vary but may involve equipment checks within the production area, monitoring of equipment from the control room or conducting process tasks for other stages of the process which do not involve diglyme. The operator does not have any direct contact with diglyme during process synthesis tasks. Therefore, the technical setup effectively prevents exposure of personnel to diglyme. Releases to the environment from this process steps are not expected due to complete containment of the process.

In the event of an emergency breakdown, a safety system is in place to assess exposure and to ensure that the appropriate measures are in place ensuring no impact to human health and/or environment.

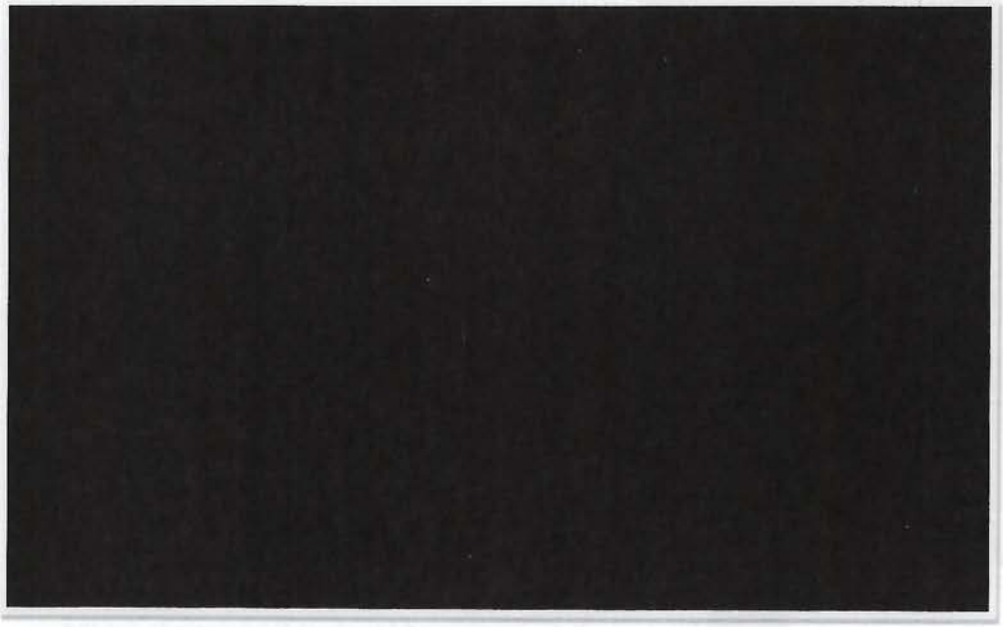

Figure 2: production equipment at [redacted], with closed synthesis reactor

Product isolation on [redacted] filter

The product solution is transferred after the chemical synthesis from the synthesis reactor to the precipitation reactor [redacted] within in a closed piping system. In the precipitation reactor a suspension is formed by adding water to the reaction mass. This suspension is transferred via a pipe system into a [redacted] filter. The [redacted] filter is placed in a completely housed area (figure 3) and vapours are exhausted at several locations to a scrubber system. The wet intermediate is isolated within the closed [redacted] filter and the mother liquor containing [redacted]% of diglyme is sucked of via pipeline and sent to waste tank [redacted].

Figure 3: [redacted] filter in its own housing within production building [redacted]

During the filtration process the [redacted] filter needs to be opened for short time periods for the operator to spread the wet filter cake to ensure a proper filling of the [redacted] This must be done 2-3 times per batch for a period of 5 minutes, the overall filtration step lasts [redacted] hours on average. At that time the diglyme assay in the liquid phase is [redacted]%. After the batch is transferred completely to the "[redacted]", the filter cake is washed efficiently with water and the diglyme content is reduced to < [redacted]%.

Sample taking of wet filter cake for analytical purposes

After the washing step, a sample is taken from the wet filter cake and put into a small plastic bottle. The bottle is closed and transferred from the operator to the analytical laboratory. The preparation of the sample and the measurements are carried out under a hood in an analytical laboratory in the same production building [redacted]. The operator takes the filter cake out of the bottle and places it on a tray. The tray is then transferred from the operator into an exsiccator for drying. The lab technician takes the dried product out of the exsiccator and analyses the residual water content and the inherent viscosity of the final product.
After confirmation of the product specifications the wet cake is transferred from the operator manually from the [redacted] filter to trays (figure 4).

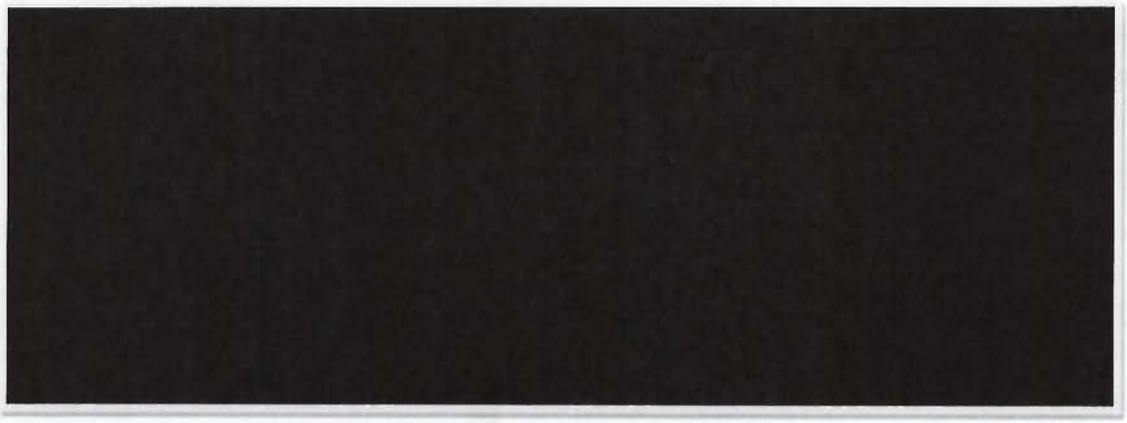

Figure 4: handling of the precipitated product at the [redacted] in its own housing [redacted]

The trays are [redacted] transferred to the neighbouring drying room and the trays are put into vacuum ovens. During all this process steps the operator is wearing PPE and no non-protected operators may enter the area.

Personal protective equipment during the filtration process consists of:

a) Respiratory PPE: air from independent respiratory system (3M™ Versaflo™ S-657 with Versaflo V500)
b) Skin PPE: Suitable gloves (VersaTouch Orange Supraweight 87-370, including Ansell Barrier 5-layer underglove) and protective clothing including safety shoes
c) Eye protection: provided by respiratory system (Versaflo)

The trays are then transferred from the operator into the vacuum oven for drying (figure 5), the last solvent traces evaporated within the closed oven system are absorbed in a scrubber system at the production facility [redacted].

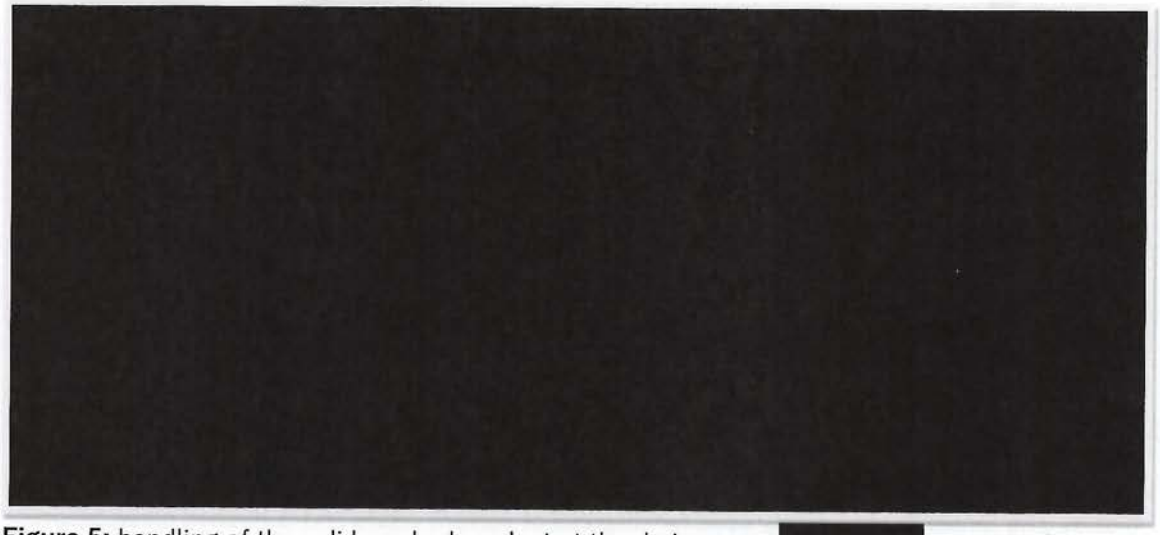

Figure 5: handling of the solid washed product at the drying oven [redacted], operator has its own air breath supply

The dried product is finally taken out of the vacuum oven from the operators and discharged into drums using a semi-automated filling line. The operator is wearing PPE as described above for this last process step. The content of Diglyme in the final product is below the detection limit (< [redacted] %).

Waste handling

Transfer of the bulk solvent waste (containing diglyme in [redacted] %) from a closed waste storage tank to

a) the incineration plant on site

b) or railway tankers for transport to an incineration plant which is not on site.

At present, the entire amount of wastewater is given to [redacted] AG for subsequent incineration. [redacted] The remaining amount will be incinerated by [redacted]. Irrespective of the process, the entire amount of wastewater is incinerated. Only traces of Diglyme from the scrubber do get into the river Rhine. The effluent of the respective sewage treatment plant (ARA Rhein) is monitored.

The waste tank [redacted], which is inertised with nitrogen and exhaust vapours are directed to onsite incineration receives only waste water streams containing diglyme in approximately [redacted] % (final concentration).

a) From tank [redacted] the diglyme containing waste is transferred to another waste tank [redacted] which is directly connected to the incineration plant on the site. The waste is mixed with other streams and incinerated. Sampling of the waste stream (~[redacted]% of Diglyme) from Tank [redacted] [redacted] [redacted] is done outdoor. The operator is wearing PPE.

   - Skin PPE: Suitable gloves (**Uvex Rubiflex NB 35S**) and protective clothing including safety shoes
   - Eye protection: protective goggles are worn.

b) From tank [redacted], railway tankers (~50 m³) are charged via pipe. The liquid waste is transferred to a railway tanker and sent to off-site incineration as hazardous waste approximately 4 times per month. The tanker is exclusively used for disposal of solvent waste and is flushed clean before being filled. Railway tanker loading from waste tank [redacted] is carried out in the tanker laydown

area. The transfer pipe and the ventilation pipe are coupled via safety couplings to the railroad tanker. The off-gas is sent to incineration. The likelihood of exposure during the various phases of waste transfer is assessed as follows: 1) Coupling of the pipe with the tanker hatch is not associated with any exposure since the solvent waste is still enclosed in tank [redacted]; 2) Automated solvent transfer, controlled remotely; 3) Upon termination of waste transfer, by decoupling of the safety valve the transfer pipe and the tanker are automatically closed. No samples are taken; no open handling must be done during the discharging process. Therefore, the likelihood of contamination for the operator is very low. The operator is wearing PPE.

- Skin PPE: Suitable gloves (**Uvex Rubiflex NB 35S**) and protective clothing including safety shoes.
- Eye protection: protective goggles are worn.

Tonnage information

The current annual consumption of diglyme as process solvent is calculated at [redacted] tonnes/year, [redacted] As a worst-case approach, the exposure was calculated for [redacted] t annual use.

Tonnage supplied per market sector

Not relevant for this application; this CSR has been prepared in the context of an individual application for authorisation of one specific use of diglyme. The current CSR covers only this particular use hence market sector-wide tonnages need not be considered.

9.0.2 Overview of exposure scenarios

The format of this CSR follows the current ECHA template for CSRs.

Table 1. Overview on exposure scenarios and coverage of substance life cycle

ES number	Short description of exposure scenario	Resulting life cycle stage				Sector of use (SU)	Process Category (PROC)	Product Category (PC)	Article Category (AC)	Environmental Release Category (ERC)	Volume (tonnes)
		Manufacture	Formulation	End use	Service life (for articles)						

				Industrial	Professional	Consumer							
9.1	Solvent for Production of a Fine Chemical			x				9	1, 8b, 9, 15			7	[redacted]

9.0.3 Introduction to the assessment

Exposure scenario 9.1 has been calculated using EasyTRA 4.3.0. EasyTRA uses algorithms on the basis of the latest versions of the ECHA REACH Guidance chapters R12 (as of 2015), R14, R15, and R16 (as of 2016) and EUSES®. EasyTRA is a graphical user interface which works in compliance with ECETOC® Targeted Risk Assessment 3 (as of July 2012; for detailed information see ECETOC Technical Report No. 114) for the calculation of worker and consumer exposure and complies with EU TGD 2003 Risk Assessment Spreadsheet Model 1.24a for the environmental exposure (see ECHA REACH Guidance chapter R16 A.16-5.2). Results obtained by EasyTRA are routinely validated against the results obtained by performing the same calculations with the original tools.

Details on used Targeted Risk Assessment:

Exposure assessment in EasyTRA follows a tiered approach, offering increasingly sophisticated refinements at later tiers to adapt the scenarios to real-life situations. The Tier 1 assessments (reduced number of parameters, conservative results) refer to ECETOC TRA v3, 2012 for the consumer, worker and environmental exposure assessment. The Tier 2 assessments refer to ConsExpo 4.1 model for consumer exposure assessment or EU TGD 2003 Risk Assessment Spreadsheet Model 1.24a for the calculation of environmental exposure (EUSES), including full access to all EUSES parameters as a third step in the refinement. EasyTRA can also perform a qualitative assessment, following ECHA Guidance Part E or externally calculated values can be considered. EasyTRA offers the options to generate user defined spERCs, article and product categories as a first refinement in the exposure calculations, before switching to higher Tier tools. The following modifications are possible for the worker exposure assessment, that are already suggested in the ECETOC TRA guidance document TR114: Factor for Peak exposure, use of the exact concentration instead of ECETOCs category approach, and use of the exact process duration instead of ECETOCs category approach. In addition, the exact value for the effectiveness of specific types of respiratory protection can be entered. Values originate from EU standards DIN EN136, EN140, EN143, EN149, EN12941, EN12942. All deviations require mandatory justifications,

which are documented in the CSR to assure full transparency of the calculations and underlying assumptions.

Unless stated otherwise, Simple Treat 4.0 has been used for modelling the biological sewage treatment plant (STP) according to ECHA Guidance on information requirements and Chemical Safety Assessment, Chapter R.16: Environmental exposure assessment, Version 3.0. The model describes the current state of the art of municipal STP in Europe and has been documented and validated: Struijs J (2014) SimpleTreat 4.0: a model to predict fate and emission of chemicals in wastewater treatment plants: Background report describing the equations. RIVM Report 601353005. RIVM, Bilthoven The Netherlands and Struijs J (2015) Application of SimpleTreat 4.0 in European substance regulations. UBA Report TEXTE 13/2015. Umweltbundesamt, Dessau, Germany). The outcome of the sewage treatment plant model is reported in terms of biological elimination and fractions directed to air, sludge and the effluent from the STP. The fractions have been used for subsequent estimation of different PECs.

9.0.3.1 Reference values used for the quantitative risk assessment

Table 2. Reference values (DNEL / PNEC)

Route / Compartment	Value
Human health	
Worker - inhalation long-term systemic	1.68 mg/m³
Worker - dermal long-term systemic	0.240 mg/kg bw/day
Environment	
STP	50 mg/L
Freshwater	6.4 mg/L
Freshwater sediment	27.4 mg/kg dwt
Marine water	0.640 mg/L
Marine water sediment	2.74 mg/kg dwt
Terrestrial compartment	1.72 mg/kg dwt
Man via environment	1.04 mg/kg bw/day
Secondary poisoning	2.77 mg/kg food

Table 3. Physical/chemical properties

Property	Value
Molecular weight	134.18 g/mol
Vapour pressure	60 Pa
Water solubility	9.40E5 mg/L
logKow	-3.60E-1
Chemical class for QSAR	Predominantly hydrophobics
Biodegradability	inherently biodegradable, fulfilling criteria

9.0.3.2 Worker assessment

Diglyme was included into Annex XIV of the REACH Regulation (the list of substances subject to authorisation) due to its intrinsic properties as being toxic to reproduction (classification as Repr 1B, H360FD – may damage fertility; may damage the unborn child.). Following Regulation (EC) No 1907/2006, Article 62(4)(d), the CSR supporting an application for authorisation needs to cover only those risks arising from the intrinsic properties specified in Annex XIV. The dominating health effects resulting from the intrinsic hazardous properties of diglyme are:

- Impairment of male reproductive organs
- Developmental toxicity, most notably increased incidence of resorption and a higher risk of major malformations

The DNELs presented in Table 2 were derived by the Member State Competent Authorities (MSCAs) responsible for the Annex XV dossier on the basis of the developmental and reproductive toxicity studies in which the above effects were identified. Based on the dose-response relationships, developmental toxicity was identified as the most critical effect. Therefore, the DNELs are considered to be sufficiently protective against the critical effects and also against any other health effects, if relevant.

Estimates of inhalation exposure were calculated using ECETOC 3 (as implemented in EasyTRA 4.2). Tier 2 dermal exposure modelling, where suitable, was performed using the Advanced Reach Tool (ART). In case measured values were available, these values were given preference over modelled values. The measured values were corrected for PPE and duration according to ECETOC, where applicable.

Estimation of dermal exposure was performed using ECETOC 3 (as implemented in EasyTRA 4.2) by default, being the standard model for dermal exposure assessment under REACH. Tier 2 dermal exposure modelling, where suitable, was performed using RISKOFDERM v2.1. ECETOC TRA returns extremely conservative dermal exposure estimates with these PROCs, not adequately reflecting substance properties and the level of protection provided by the operational conditions and risk management measures in place. RISKOFDERM, by contrast, allows more targeted modelling of the level of dermal contact and is an accepted tool collaboratively developed by several EU member states' competent authorities. With the remaining scenarios, in consideration of the consistently high level of occupational safety in place during the handling of Diglyme, the relatively simplistic approach of ECETOC TRA is considered to be appropriate.

The following effectiveness values are assumed for the use of chemically resistant gloves:
Use of suitable gloves: 80%; Use of suitable gloves in combination with basic employee training: 90%; Use of suitable gloves in combination with specific activity training: 95%; Use of suitable gloves in combination with intensive management supervision controls: 98%. The use of 98% is in line with ECETOC Technical report 131 and ECHA guidance on Information Requirements and Chemical Safety Assessment Chapter R.14: Occupational exposure assessment)

9.0.3.3 Environmental assessment

Special considerations for the calculation of the environmental part

Currently, [redacted] of Diglyme are used as solvent per year, but an increase to an annual use of [redacted]t is planned. Following an extreme worst-case approach, the environmental assessment was performed with [redacted]t annual use.

Diglyme is not classified for the environment. The respective LC50/EC50/NOEC values are well above the regulatory relevant trigger values. In a chronic toxicity study towards Daphnia magna a NOEC of 320 mg/L was determined which was used for the derivation of the respective PNEC values. In general, no adverse effects in the environment are to be expected.
Nevertheless, an environmental exposure assessment has been conducted for diglyme with site-specific data from the production site in Schweizerhalle, Switzerland.
The use of diglyme as process chemical results in approximately [redacted] T of wastewater per year. At present, the entire amount of wastewater is given to [redacted] AG for subsequent incineration. In the future, a new process is supposed to be established to split the amount of wastewater. A maximum amount of [redacted] T will then be transported [redacted] for incineration. First trials have taken place. The remaining amount will be incinerated by [redacted] AG. Irrespective of the process, the entire amount of

wastewater is incinerated. Only traces of Diglyme from the scrubber do get into the river Rhine. The effluent of the respective sewage treatment plant (ARA Rhein) is monitored.

With the exception of the below-discussed parameters the environmental exposure assessment has been conducted with the default parameters of ERC 7 which are in general very conservative. Figure 6 depicts an overview of the ARA Rhein with indications of the monitoring site of diglyme and the separate evaluation of the STP (see text below for details).

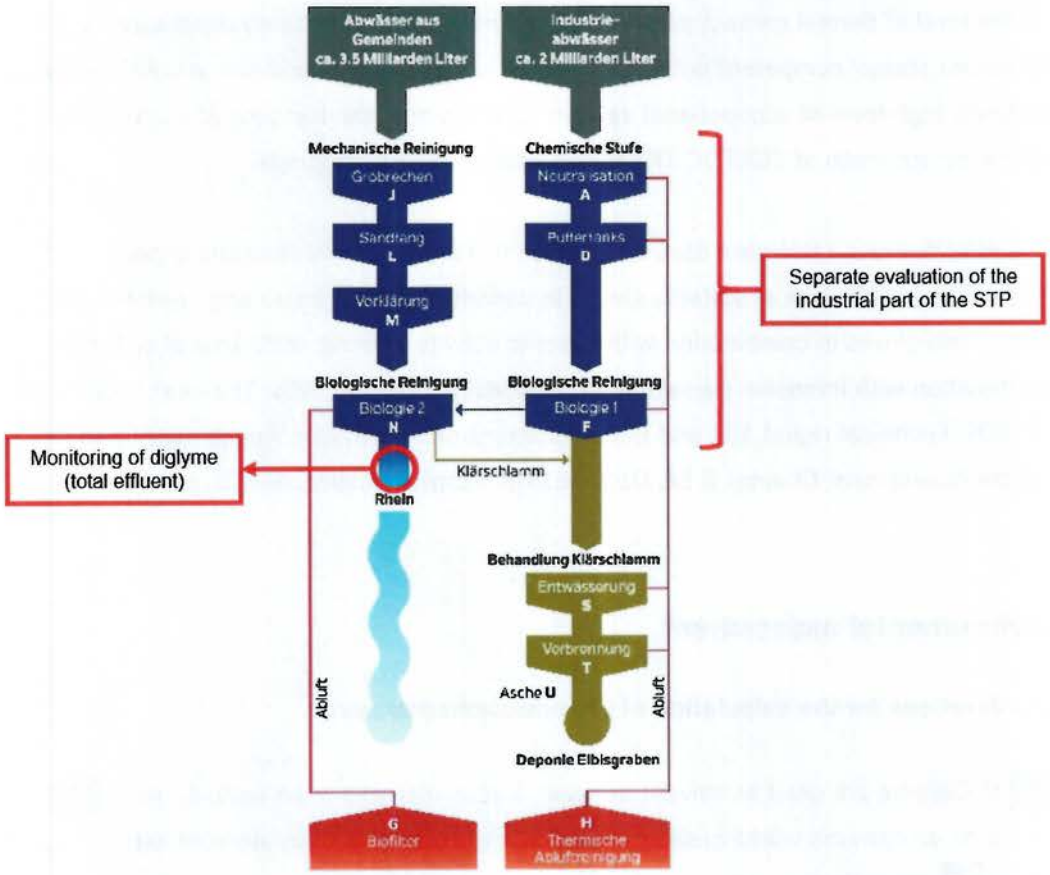

Figure 6: Overview of the ARA Rhein with indications were diglyme is monitored and the separate evaluation of the industrial part of the STP. STP schematic is taken from the webpage of ARA Rhein (https://www.ararhein.ch; accessed on January 24th, 2019).

Special considerations for the risk of the sewage treatment plant ARA Rhein

The concentration of diglyme in the total effluent of the ARA Rhein is constantly monitored. In the 3rd quarter 2018, the max concentration was 55 µg/L. The ARA Rhein treats both the communal effluents of the surrounding communities with a population equivalent of 50'000 and the industrial effluents of the surrounding industries representing a population equivalent of 450'000. These two effluent streams are treated separately until the biological stage. From there the combined treated wastewater is discharged into the river Rhine. The monitoring of diglyme is conducted in the combined effluent stream which is relevant for the subsequent mixing in the river. As the communal and industrial effluent streams are treated separately the concentration of diglyme in the industrial influent is of course higher compared to the total effluent due to the differing

amounts of water. The ratio of industrial effluent to the total amount of effluent which is finally discharged is approx. 4.5 (Table 4).

Table 4: Effluents and ratio industrial effluent to total effluent for Q1 to Q3 2018 of ARA Rhein (data taken from the final listing for the settlement). Effluent values are given in m³.

		Q1 2018	Q2 2018	Q3 2018
Industrial effluents	Company 1	22000	23000	29000
	BASF	17000	17000	19000
	Company 2	33000	26000	21000
	Company 3	72000	80000	48000
	Company 4	5000	4000	4000
	Company 5	119000	114000	107000
∑ industrial effluents		268000	264000	228000
Communal effluent (Canton)		974000	846000	715000
∑ industrial + communal		**1242000**	**1110000**	**943000**
Ratio industrial effluent / total effluent		**4.6**	**4.2**	**4.1**

The concentration of 55 µg/L diglyme in the total effluent was corrected by a factor of 4.5 to approximate the concentration in the industrial influent (55 µg/L * 4.5 ≈ 250 µg/L). As the PNEC STP was determined to be 50 mg/L (chapter 9.0.1, Table 1; EC50 = 5000 mg/L; assessment factor 100) the RCR for the industrial part of the sewage treatment plant is clearly below 1. An inhibition of the degradation activity of activated sludge by diglyme can therefore be ruled out.
As worst case, the split of industrial and communal effluent was not further accounted for in the subsequent exposure assessment. It is only described here for reasons of transparency.

Concentration in the local effluent

Trace amounts of diglyme may be transported *via* the wastewater stream to the local STP (ARA Rhein). The ARA Rhein treats both industrial wastewater and communal wastewater. The concentration of diglyme (among other substances) is constantly monitored in the effluent of the STP. The quarterly report of the ARA Rhein (3rd quarter; Quartalsbericht ARA Rhein 03/2018, 12.11.2018) states a max concentration of 55 µg/L (Figure 7). This concentration converted to kg/m³ (not the lower average value of 41 µg/L) was used in the exposure calculations (EUSES variable Clocal.eff). As it represents the max value it can be regarded as representative worst case.

GESAMTAUSLAUF	Einheit	Anzahl Werte [3]	Nachweis-grenze	Min. [1]	Max. [1]	Mittel [1]	Fracht kg/Quartal
NOVARTIS [2] / BASF							
1-Brom-3-chlorpropan	mg/l	3	0.01		< 0.01		
Chlorimipraminbase (Anafranil)	mg/l	3	0.01		< 0.01		
Diethylenglykoldimethylether	mg/l	3	0.01	0.026	0.055	0.041	61.6

Figure 7: Concentration of diglyme in the effluent of the ARA Rhein.

Effluent discharge rate

Furthermore, instead of the default value of 2000 m³/d the site-specific discharge rate of the ARA Rhein was used. This value was also taken from the quarterly report of the ARA Rhein (3rd quarter; Quartalsbericht ARA Rhein 03/2018, 12.11.2018). The report lists the influent rates to the STP per quarter. It can be assumed that the effluent rates correspond to the influent rates. As worst case, the lowest value (in this case from the 3rd quarter 2018) was used for the subsequent calculation of the dilution factor. Taking the total amount of wastewater for the 3rd quarter 2018 of 1'093'000 m³ and dividing it by the amount of days for the 3rd (92d) results in a value of 11'880 m³/d (11'880'435 L/d).

Parameter (Summe aller Zuläufe)	**Einheit**	**1. Quartal**	**2. Quartal**	**3. Quartal**	**4. Quartal**	**Quartals-Mittel Vorjahr**
Abwasser-Menge	1'000 m³	1'342	1'227	1'093		1318
Aciditäts-Fracht	Tonnen	375	363	230		442
TOC-Fracht	Tonnen	953	945	548		902

Figure 8: Influent rates of the ARA Rhein. Data from the quarterly report 03/2018 (3rd quarter; Quartalsbericht ARA Rhein 03/2018, 12.11.2018).

River flow rate

The site-specific river flow rate was used for the assessment. The data has been taken from the webpage of the Federal Office for the Environment FOEN (https://www.hydrodaten.admin.ch/de; accessed on January 23rd, 2019). The nearest monitoring station for hydrological data is located in Rheinfelden with the ID 2091. The annual discharge data from this station (Fig. 9) has been used to determine the low-flow rate (10th percentile) to account for fluctuating flow rates throughout the year (36'720'000 m³/d). This is in line with ECHA's Guidance on information requirements and Chemical Safety Assessment, Chapter R.16: Environmental exposure assessment (version 3.0, February 2016).

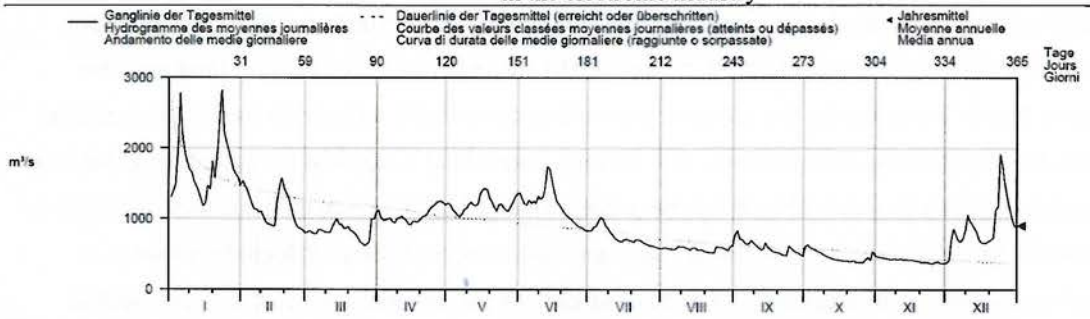

Figure 9: Discharge rate of the river Rhine from the monitoring station Rheinfelden (ID 2091). Data accessed on Januar 23rd, 2019. https://www.hydrodaten.admin.ch/en/2091.html

According to the Federal Office of Meteorology and Climatology MeteoSwiss, 2018 was one of the driest years since monitoring. The annual precipitation was only 80 to 95% of the values from 1981-2010 (Fig. 10; MeteoSchweiz 2019: Klimabulletin Jahr 2018. Zürich). Therefore, the river flow rate which was used in the current assessment can clearly be regarded as worst case.

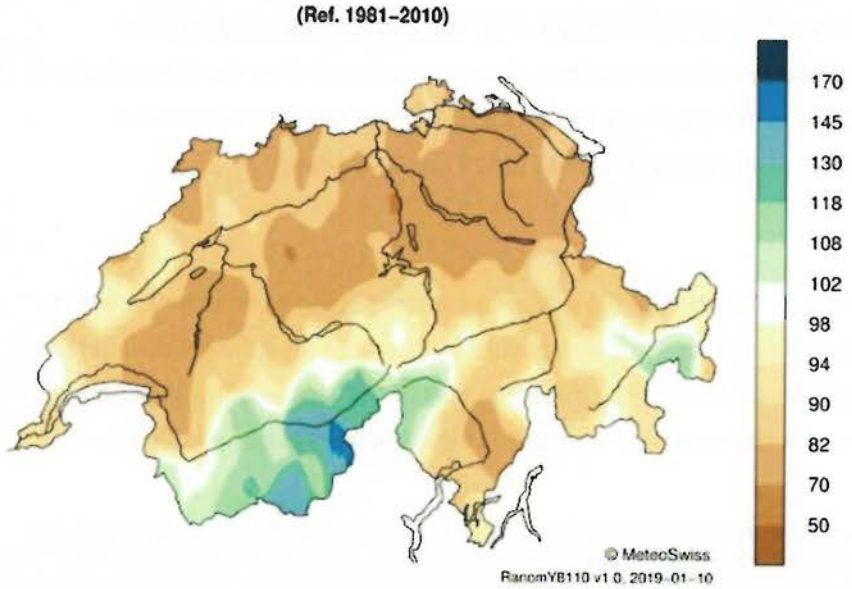

Figure 10: Annual precipitation in % of the norm (MeteoSchweiz 2019: Klimabulletin Jahr 2018. Zürich).

According to ECHA's R.16 Guidance Document the site-specific effluent discharge and the river flow rate can be used to calculate the dilution factor with the following equation:

$$DILUTION = \frac{EFFLUENT_{stp} + FLOW}{EFFLUENT_{stp}}$$

For the current case, a dilution factor of 3091.8 can be derived from the site-specific values. It must be noted that with the assumption of complete mixing of the effluent in the surface water, no account is taken of the fact that in reality higher concentrations will occur in the mixing zone.

For situations with relatively low dilution factors, this mixing zone effect can be accepted. For situations with very high dilution factors, however, the mixing zones may be very long and the overall area that is impacted by the effluent before it is completely mixed can be very substantial. Therefore, for site-specific assessments, the dilution factor that is applied for calculating the local concentration in surface water should not be greater than 1000. In line with these assumptions, a dilution factor of 1000 was used for the subsequent calculation of the PEC local.freshwater. It needs to be pointed out that approx. 7 km downstream of the production site the hydroelectric power station KWB Birsfelden leads to a thorough mixing of the effluent stream with the river water. Therefore, a dilution factor of 1000 clearly represents a worst-case assumption.

Release to soil – fate of the sludge resulting from the tertiary sewage treatment

No direct release to soil occurs. The sludge of the tertiary sewage treatment is completely incinerated and no discharge onto soils occur.

Release to air

The release of diglyme to air is not monitored. For low-boiling substances the regulations according to LRV-1 (Luftreinhalteverordnung) are met. It can be assumed that the concentrations of higher boiling substances are within these parameters. For the environmental exposure assessment, the conservative default release factor of ERC 7 was used (5%).

Summary

The adapted parameters for the calculation of the environmental exposure assessment are listed in Table 5 below. All other parameters used in the exposure assessment are conservative default values. As mentioned above, the situation for the industrial part of the ARA Rhein was separately assessed. An overview of the risk management measures of the site can found in Table 6.

Table 5: Adapted parameters used for the calculation of the environmental exposure assessment.

Parameter	Value
Clocal.eff	55 µg/L *
Effluent discharge rate	11'880'435 L/d
River flow rate	36'720'000 m³/d
Reduction of sludge to soil	100% (complete incineration of the sludge)

* For the calculation of the PEC regional freshwater the default release factor of 5% of ERC 7 was used.

Table 6: The Risk Management Measure and Operational Conditions for the safe handling and use of diglyme are summarized in the below table.

Task (ERC, PROC)	Annual amount per site (T/a)	Technical RMMs	Organisational RMMs	PPE	Effectiveness of wastewater and waste air treatment (for ERC)	Release factors: water, air and soil (for ERC)	Detailed info in CSR (section)
ERC 7	[redacted]	Completely closed system; closed piping; wastewater incineration	Automated operation (remote control) by trained personnel	Not applicable	Not applicable – the entire amount of wastewater is incinerated. Only trace amounts reach the river Rhine.	Water: ERC default of 5% and Clocal.eff: 55µg/L Air: ERC default of 5% Soil: ERC default of 5% (no sludge to soil)	9.1.1
PROC 8b (Charging)		Local Exhaust Ventilation	Specific activity training; Duration: 5 min (attachment of lance); 60 min (charging); Frequency: every 2nd day	Full Mask (Jupiter system, 3M) with filter type ABEK P3. Suitable gloves (KCL Vitoject 890) and protective clothing including safety shoes.			9.1.2
PROC 1 (Chemical Synthesis)		Completely closed reactor; Remote control of all processes	Specific activity training	Protective clothing including safety goggles.			9.1.3
PROC 9 (Sampling)		Local Exhaust Ventilation during sampling; Closed sampling box; Transport of sample jar to laboratory sealed and in bottle carrier	Specific activity training; Duration: < 15 min	Air from independent respiratory system (3M™ Versaflo™ S-657 with Versaflo V500). Suitable gloves (VersaTouch Orange Supraweight 87-370, including Ansell Barrier 5-layer underglove) and protective clothing including safety shoes.			9.1.4
PROC 15 (Laboratory)		Local Exhaust Ventilation (fume hood)	Specific activity training; Duration: < 4h	Suitable gloves and protective clothing.			9.1.5
PROC 8b (Product Isolation)		Local Exhaust Ventilation	Specific activity training; Duration: < 4h	Air from independent respiratory system (3M™ Versaflo™ S-657 with Versaflo V500). Suitable gloves (VersaTouch Orange Supraweight 87-370, including Ansell Barrier 5-layer underglove) and protective clothing including safety shoes.			9.1.6
PROC 8b (Product Transfer)		Local Exhaust Ventilation	Specific activity training; Duration: < 60 min	Air from independent respiratory system (3M™ Versaflo™ S-657 with Versaflo V500). Suitable gloves (VersaTouch Orange Supraweight 87-370, including Ansell Barrier 5-layer underglove) and protective clothing including safety shoes.			9.1.7
PROC 8b (Waste Water Sampling)			Outdoors; Specific activity training; Duration: 2 min via valve	Suitable gloves (Uvex Rubiflex NB 35S) and protective clothing including safety shoes; Protective goggles			9.1.8
PROC 8b (Waste Transfer)			Outdoors; Specific activity training; Duration: 5 min; attachment and detachment of pipe)	Suitable gloves (Uvex Rubiflex NB 35S) and protective clothing including safety shoes; Protective goggles			9.1.9

9.1 Scenario 1: Solvent for Production of a Fine Chemical

Personnel involved:

[redacted] full-time employees are directly involved in the scenarios described in this chapter (see the table below for exact figures for each contributing scenario). All directly involved personnel are male.

[redacted] additional full-time employees are indirectly involved, working in the same building but in different rooms. These employees are not involved during open handling of Diglyme, during charging or discharging or during drying of the final product. Measures have been taken to prevent accidental entrance of non-involved employees into rooms where Diglyme or products containing Diglyme are beings handled. Instructions are in place that further prevent accidental involvement to the steps described below.

This scenario is described by the following combinations of use descriptors. The corresponding contributing scenarios are described in the respective subchapters.

An overall exposure scenario may be described by a number of contributing scenarios which may be subdivided into environmental exposure, worker exposure and consumer exposure.
The following scenarios contribute to the scenario *Solvent for Production of a Fine Chemical.*

The corresponding release to the environment, exposure of workers and consumers resulting from these contributing scenarios is summarized in chapter 10.1 ff.

Table 4. Description of ES 1

Free short title	Solvent for Production of a Fine Chemical
Systematic title based on use descriptor	ERC 7; PROC 8B, 1, 9, 15
Name of contributing environmental scenario and corresponding ERC	ERC 7 Industrial use of substances in closed systems

Name(s) of contributing worker scenarios and corresponding PROCs	PROC 8b - Transfer of chemicals from/to vessels/ large containers at dedicated facilities *(Diglyme charging into Fine Chemical synthesis at production site)* *Number of involved personnel during this contributing scenario: directly involved*:* [redacted] *indirectly involved**:* [redacted] ** regular working during this scenario* *** working in the same building but in different rooms* PROC 1 - Use in closed process, no likelihood of exposure *(Synthesis of a fine chemical)* *Number of involved personnel during this contributing scenario: directly involved:* [redacted] *indirectly involved:* [redacted] PROC 9 - Transfer of chemicals into small containers *(Sample taking of fine chemical and transport to quality laboratory)* *Number of involved personnel during this contributing scenario: directly involved:* [redacted] *indirectly involved:* [redacted] PROC 15 - Use of laboratory reagents in small scale laboratories *(Handling at quality control laboratory)* *Number of involved personnel during this contributing scenario: directly involved:* [redacted] *indirectly involved:* [redacted]

Name(s) of contributing worker scenarios and corresponding PROCs	PROC 8b - Transfer of chemicals from/to vessels/ large containers at dedicated facilities *(Product isolation in a dedicated filter press)* *Number of involved personnel during this contributing scenario: directly involved: [redacted] indirectly involved: [redacted]* PROC 8b - Transfer of chemicals from/to vessels/ large containers at dedicated facilities *(Final Product Transfer from the drying chamber into small container)* *Number of involved personnel during this contributing scenario: directly involved: [redacted] indirectly involved: [redacted]* PROC 9 – Transfer of chemicals into small containers *(Analytical sampling: Diglyme content control in wash water from waste storage tank [redacted])* *Number of involved personnel during this contributing scenario: directly involved: [redacted]* PROC 8b - Transfer of chemicals from/to vessels/ large containers at dedicated facilities *(Partial waste transfer to road tanker)* *Number of involved personnel during this contributing scenario: directly involved: [redacted]*

9.1.1 Contributing Scenario (1) controlling environmental exposure for ERC 7

Operational conditions	
Annual site tonnage	[redacted] to/year
Daily amount used at site	[redacted] kg/day
Release times per year	[redacted] days/year
Local freshwater dilution factor	1,000
Local marine water dilution factor	100
Release fraction to air from process	5 %

Release fraction to wastewater from process	5 %
Release fraction to soil from process	5 %
Fraction tonnage to region	100 %
Fraction used at main source	100 %
STP	yes (municipal)
River flow rate	36720000 m^3/day *(justification: site specific data)*
Municipal sewage treatment plant discharge	11880435 L/day *(justification: site specific data)*
Risk management measures	
Reduction of sludge to soil	100 % *(justification: The entire sludge from the sewage treatment plant is incinerated.)*
Other modified EUSES values	
Concentration of chemical (total) in STP effluent (Clocal.eff)	0.000055 kgc.m-3 *(justification: measured data; site specific)*

9.1.2 Contributing Scenario (2) controlling industrial worker exposure for PROC 8B (PC 30)

Name of contributing scenario	8b - Transfer of chemicals from/to vessels/ large containers at dedicated facilities
Scenario subtitle	Diglyme charging into Fine Chemical synthesis at production site
Exposure type	Inhalation: Long-term systemic Dermal: Long-term systemic
Product characteristics	
Physical state	liquid
Concentration in substance	100 %
Fugacity / Dustiness	low
Frequency and duration of use	
Duration of activity	2.5 mins
Frequency of use	5 days / week
Human factors not influenced by risk management	
Exposed skin surface	960 cm^2

Other given operational conditions affecting workers exposure	
Location	indoors
Domain	industrial
Technical conditions and measures to control dispersion and exposure	
Local exhaust ventilation	yes (inhalation 95 %)
Conditions and measures related to personal protection, hygiene and health evaluation	
Protective gloves	98 %, burst-time: >4 hours (default) *(justification: For this process, gloves with an effectiveness of 98% are recommended. The 98% effectiveness is achieved and justified by specific activity training of workers in combination with intensive management supervision controls. This is in line with ECETOC Technical report 131 and ECHA guidance on Information Requirements and Chemical Safety Assessment Chapter R.14: Occupational exposure assessment).*
Respiratory protection	90 %

Dermal exposure calculation	During this scenario the only exposure possibility of the worker is during insertion of the suction lance to the Diglyme barrels. The transfer of Diglyme from the barrels to the reactor is fully automated using a closed pipe system with no exposure. Charging of Diglyme occurs every other day. Attachment and removal of the suction lance takes about 5 minutes. The potential dermal exposure during lance insertion has been calculated with "Risk of Derm 2.1" The following settings were applied: - Scenario: Mechanical Immersion of objects in liquid baths (DEO unit 5) - Distance of the worker from the source: from 30 cm to 1 m - Adequate local exhaust ventilation used: Yes - Resulting exposure rate hands (90th percentile): 176 µl/min - Cumulative duration of task during a shift: 2.5 min (5 min every other day) - Exposure loading per shift hands: 440 µl - Conversion to weight based on density: 440 µl * 0.95 mg/µl = 418 mg - Use of gloves (98 % protection); corrected exposure: 8.4 mg - Body dose (70 kg bw): 0.12 mg/kg bw/d
Inhalation exposure calculation	Inhalation exposure was not calculated since monitoring values were available. The measured Diglyme concentration from personal monitoring in the breathing zone outside respiratory protection was 0.3 mg/m³. This concentration is corrected for the use of respiratory protection: 0.3 mg/m³ x 0.1 = 0.03 mg/m³. Further adjustment for the duration of the task was done following ECETOC guideline (less than 15 minutes = 90% reduction): 0.03 mg/m³ x 0.1 (ECETOC) = 0.003 mg/m³.

9.1.3 Contributing Scenario (3) controlling industrial worker exposure for PROC 1 (PC 30)

Name of contributing scenario	1 - Use in closed process, no likelihood of exposure
Scenario subtitle	Synthesis of a Fine Chemical
Exposure type	Inhalation: Long-term systemic Dermal: Long-term systemic
Product characteristics	
Physical state	liquid
Concentration in substance	100 %
Fugacity / Dustiness	low
Frequency and duration of use	
Duration of activity	>4 hours (default)
Frequency of use	5 days / week
Human factors not influenced by risk management	
Exposed skin surface	240 cm^2
Other given operational conditions affecting workers exposure	
Location	indoors
Domain	industrial
Technical conditions and measures to control dispersion and exposure	
Local exhaust ventilation	yes (inhalation 0 %)
Conditions and measures related to personal protection, hygiene and health evaluation	
Protective gloves	Gloves APF 20 95 %
Respiratory protection	no
Dermal exposure calculation	The whole process takes place in a completely closed and automated system without sampling or other possibility for exposure. Nevertheless, calculations of exposure were performed using ECETOC TRA, although the exposure to Diglyme during synthesis of a Fine Chemical is basically zero.

Inhalation exposure calculation	The whole process takes place in a completely closed and automated system without sampling or other possibility for exposure. Nevertheless, calculations of exposure were performed using ECETOC TRA, although the exposure to Diglyme during synthesis of A fine chemical is basically zero.

9.1.4 Contributing Scenario (5) controlling industrial worker exposure for PROC 9 (PC 30)

Name of contributing scenario	9 - Transfer of chemicals into small containers (dedicated filling line)
Scenario subtitle	Sample taking of fine chemical and transport to quality laboratory *Note: Transport of the sample to the laboratory is carried out in a sealed container, therefore no exposure to residual Diglyme occurs during transport. PROC9 describes the sample taking of the fine chemical (containing residual amounts of Diglyme) in the* [redacted] *filter room and this PROC is therefore considered sufficient to describe this scenario. The sampling takes a few seconds.*
Exposure type	Inhalation: Long-term systemic Dermal: Long-term systemic
Product characteristics	
Physical state	solid
Concentration in substance	1-5%
Fugacity / Dustiness	low
Frequency and duration of use	
Duration of activity	1 min
Frequency of use	5 days / week
Human factors not influenced by risk management	
Exposed skin surface	480 cm^2
Other given operational conditions affecting workers exposure	
Location	indoors
Domain	industrial
Technical conditions and measures to control dispersion and exposure	

Local exhaust ventilation	yes (inhalation 90 %)
Conditions and measures related to personal protection, hygiene and health evaluation	
Protective gloves	Gloves APF 20 95 %
Respiratory protection	90 %
Dermal exposure calculation	The potential dermal exposure during sampling of the fine chemical containing residual amounts of Diglyme was calculated with Risk of Derm 2.1. Although the total duration of the sampling takes only a few seconds, a duration of 1 min was used for calculation as a worst-case approach. The following settings were applied: - Scenario: Filling, mixing or loading (DEO unit 1) - Quality of ventilation: Normal or good ventilation - Frequency of skin contact with the contaminant: Rare contact - Kind of skin contact with the contaminant: Light contact - Type of product: Low or moderately dusty solid - Significant amounts of aerosols or splashes generated: No - Level of automation: Manual task - Use rate of product: 0.1 kg/min - Resulting exposure rate hands (90th percentile): 0.03514 mg/min - Cumulative duration of task during a shift: 1 min - Exposure loading per shift hands: 0.03514 mg - Use of gloves (95 % protection); corrected exposure: 0.0018 mg - Correction for concentration of Diglyme (<5%): 0.00009 mg - Body dose (70 kg bw): 0.000001 mg/kg bw/d

Inhalation exposure calculation	Inhalation exposure was not calculated since monitoring values were available. The measured value from personal monitoring at the [redacted] filter under respiratory protection was 0.21 mg/m³. This concentration is adjusted for the duration of the task following ECETOC guideline (less than 15 minutes = 90% reduction): 0.21 mg/m³ x 0.1 (ECETOC) = 0.021 mg/m³

9.1.5 Contributing Scenario (6) controlling industrial worker exposure for PROC 15 (PC 30)

Name of contributing scenario	15 - Use of laboratory reagents in small scale laboratories
Scenario subtitle	Handling at quality control laboratory
Exposure type	Inhalation: Long-term systemic Dermal: Long-term systemic
Product characteristics	
Physical state	solid
Concentration in substance	1-5%
Fugacity / Dustiness	low
Frequency and duration of use	
Duration of activity	1 - 4 hours
Frequency of use	5 days / week
Human factors not influenced by risk management	
Exposed skin surface	240 cm²
Other given operational conditions affecting workers exposure	
Location	indoors
Domain	industrial
Technical conditions and measures to control dispersion and exposure	
Local exhaust ventilation	yes (inhalation 90 %)
Conditions and measures related to personal protection, hygiene and health evaluation	
Protective gloves	Gloves APF 20 95 %
Respiratory protection	No
Dermal exposure calculation	Dermal exposure was calculated with ECETOC TRA.

Inhalation exposure calculation	Inhalation exposure was calculated with ECETOC TRA.

9.1.6 Contributing Scenario (7) controlling industrial worker exposure for PROC 8B (PC 30)

Name of contributing scenario	8b - Transfer of chemicals from/to vessels/ large containers at dedicated facilities
Scenario subtitle	Product isolation in a dedicated filter press
Exposure type	Inhalation: Long-term systemic Dermal: Long-term systemic
Product characteristics	
Physical state	solid
Concentration in substance	1-5%
Fugacity / Dustiness	low
Frequency and duration of use	
Duration of activity	1 - 4 hours
Frequency of use	5 days / week
Human factors not influenced by risk management	
Exposed skin surface	960 cm^2
Other given operational conditions affecting workers exposure	
Location	indoors
Domain	industrial
Technical conditions and measures to control dispersion and exposure	
Local exhaust ventilation	yes (inhalation 95 %)
Conditions and measures related to personal protection, hygiene and health evaluation	
Protective gloves	Gloves APF 20 95 %
Respiratory protection	90 %

Dermal exposure calculation	Dermal exposure was calculated with the more conservative ECETOC model, since the scenarios implemented in Risk of Derm 2.1 are not suitable for this task. However, in consideration of the consistently high level of occupational safety in place during the handling of Diglyme, the relatively simplistic approach of ECETOC TRA is considered sufficiently cover this scenario.
Inhalation exposure calculation	Inhalation exposure was not calculated since monitoring values were available. The Diglyme concentration from personal monitoring at the [redacted] filter under respiratory protection was 0.21 mg/m³. This value was measured over a time period of 43 minutes, most closely reflecting the average exposure time during this task. This concentration is adjusted for the duration of the task following ECETOC guideline (1h - 4h = 40% reduction): 0.21 mg/m³ x 0.6 (ECETOC) = 0.13 mg/m³

9.1.7 Contributing Scenario (8) controlling industrial worker exposure for PROC 8B (PC 30)

Name of contributing scenario	8b - Transfer of chemicals from/to vessels/ large containers at dedicated facilities
Scenario subtitle	Final Product Transfer from the drying chamber into small container
Exposure type	Inhalation: Long-term systemic Dermal: Long-term systemic
Product characteristics	
Physical state	solid
Concentration in substance	[redacted]
Fugacity / Dustiness	medium
Frequency and duration of use	
Duration of activity	15 min – 1 hour
Frequency of use	5 days / week
Human factors not influenced by risk management	
Exposed skin surface	960 cm²

Other given operational conditions affecting workers exposure	
Location	indoors
Domain	industrial
Technical conditions and measures to control dispersion and exposure	
Local exhaust ventilation	yes (inhalation 95 %)
Conditions and measures related to personal protection, hygiene and health evaluation	
Protective gloves	Gloves APF 20 95 %
Respiratory protection	90 %

Dermal exposure calculation	Transfer of the final product from the drying chamber to drums occurs at a semi-automated filling line. The trays from the drying chamber containing the final product are emptied [redacted] into barrels. This task takes [redacted] for one production batch. [redacted] Dermal exposure was calculated using "Risk of Derm 2.1". The following settings were applied: - Scenario: Filling, mixing or loading (DEO unit 1) - Quality of ventilation: Normal or good ventilation - Frequency of skin contact with the contaminant: More than rare contact - Kind of skin contact with the contaminant: more than light contact - Type of product: Low or moderately dusty solid - Significant amounts of aerosols or splashes generated: No - Level of automation: Manual task - Use rate of product: 1 kg/min [redacted] - Body dose (70 kg bw): 0.0012 mg/kg bw/d
Inhalation exposure calculation	Inhalation exposure was calculated with ECETOC TRA.

9.1.8 Contributing Scenario (8) controlling industrial worker exposure for PROC 9 (PC 30)

Name of contributing scenario	9 - Transfer of chemicals into small containers (dedicated filling line)
Scenario subtitle	Analytical sampling (Diglyme content control in wash water) from waste storage tank [redacted]

Exposure type	Inhalation: Long-term systemic Dermal: Long-term systemic
Product characteristics	
Physical state	liquid
Concentration in substance	<3%
Fugacity / Dustiness	low
Frequency and duration of use	
Duration of activity	1 min
Frequency of use	5 days / week
Human factors not influenced by risk management	
Exposed skin surface	480 cm^2
Other given operational conditions affecting workers exposure	
Location	outdoors (30%)
Domain	industrial
Technical conditions and measures to control dispersion and exposure	
Local exhaust ventilation	no
Conditions and measures related to personal protection, hygiene and health evaluation	
Protective gloves	Gloves APF 20 95 %
Respiratory protection	no

Dermal exposure calculation	Prior to on-site incineration a small sample is taken from the waste water tank for analytical purposes using a safety valve. The content of Diglyme in the waste water is about 3%. The potential dermal exposure was calculated using "Risk of Derm 2.1". Although the total duration of the sampling takes only a few seconds, a duration of 1 min was used for calculation as a worst-case approach. The following settings were applied: - Scenario: Filling, mixing or loading (DEO unit 1) - Quality of ventilation: Normal or good ventilation - Frequency of skin contact with the contaminant: Rare contact - Kind of skin contact with the contaminant: Light contact - Type of product: Liquid - Significant amounts of aerosols or splashes generated: No - Level of automation: Manual task - Use rate of product: 1 l/min Resulting exposure rate hands (90th percentile): 8.7 µl/min Cumulative duration of task during a shift: 1 min Exposure loading per shift hands: 8.7 µl = 8.7 mg Use of gloves (95 % protection); corrected exposure: 0.435 mg Correction for concentration of Diglyme (<3%): 0.013 mg Body dose (70 kg bw): 0.0002 mg/kg bw/d

Inhalation exposure calculation	The potential exposure by inhalation was calculated with the Advanced Reach Tool (ART) v1.5 The following settings were applied: Duration: 1 min Emission sources: Near field Process temperature: Room temperature Vapor Pressure: 100 Pa Liquid mole fraction: small Activity coefficient: 1 Activity class: Falling liquids Situation: Transfer of liquid product with flow of 0.1 - 1 l/minute Loading Type: Splash loading, where the liquid dispenser remains at the top of the reservoir and the liquid splashes freely Process fully enclosed: No Effective housekeeping practices in place: Yes Work area: Outdoors Source located close to buildings: Yes Primary localized controls: no (0.00 % reduction) Secondary localized control: no (0.00 % reduction) The predicted air concentration (90th percentile) in a worker's personal breathing zone outside of any Respiratory Protection Equipment (RPE) is 0.00016 mg/m³.

9.1.9 Contributing Scenario (9) controlling industrial worker exposure for PROC 8B (PC 30)

Name of contributing scenario	8b - Transfer of chemicals from/to vessels/ large containers at dedicated facilities
Scenario subtitle	Partial waste transfer to road tanker
Exposure type	Inhalation: Long-term systemic Dermal: Long-term systemic
Product characteristics	
Physical state	liquid
Concentration in substance	<3%
Fugacity / Dustiness	low

Frequency and duration of use	
Duration of activity	5 min
Frequency of use	5 days / week
Human factors not influenced by risk management	
Exposed skin surface	960 cm^2
Other given operational conditions affecting workers exposure	
Location	outdoors (30%)
Domain	industrial
Technical conditions and measures to control dispersion and exposure	
Local exhaust ventilation	no
Conditions and measures related to personal protection, hygiene and health evaluation	
Protective gloves	Gloves APF 20 95 %
Respiratory protection	no

Dermal exposure calculation	In the future, one part of the waste water will be transferred from the waste water tank via pipe to railway tankers for transportation for off-site incineration. Trials of this process have already taken place. The transfer pipe and the ventilation pipe are coupled via safety couplings to the railroad tanker. The off-gas is sent to incineration. Coupling of the pipe with the tanker hatch is not associated with any exposure since the solvent waste is still enclosed in tank [redacted]. The transfer itself is automated and controlled remotely without exposure possibilities. Upon termination of waste transfer, by decoupling of the safety valve the transfer pipe and the tanker are automatically closed. Nevertheless, a small chance for exposure the residual waste water is possible. This step is therefore taken into consideration for exposure calculation. Dermal exposure was calculated using "Risk of Derm 2.1". The following settings were applied: - Scenario: Filling, mixing or loading (DEO unit 1) - Quality of ventilation: Normal or good ventilation - Frequency of skin contact with the contaminant: Rare contact - Kind of skin contact with the contaminant: Light contact - Type of product: Liquid - Significant amounts of aerosols or splashes generated: No - Level of automation: Manual task - Use rate of product: 1 L/min (worst case assumption for contaminated objects) Resulting exposure rate hands (90th percentile): 8.7 µl/min Cumulative duration of task during a shift: 5 min Exposure loading per shift hands: 8.7 µl = 43.5 mg Use of gloves (95 % protection); corrected exposure: 2.175 mg Correction for 3 % diglyme content in solvent waste: 0.065 mg Body dose (70 kg bw): 0.0009 mg/kg bw/d

Inhalation exposure calculation	During the automated transfer of the waste water from the storage tank to the railroad tanker, no exposure occurs. During removal of the pipe from the safety coupling after transfer could potentially could potentially be associated with exposure to residuals. This step is therefore assessed using the Advanced Reach Tool (ART) v1.5. The following settings were applied: Emission sources: Near field Duration: 5 min Process temperature: Room temperature Vapor Pressure: 100 Pa Liquid mole fraction: small Activity coefficient: 1 Activity class: Handling of contaminated objects Situation: Activities with treated/contaminated objects (surface 0.3-1 m^2) Contamination level: Contamination > 90 % of surface (extreme worst case) Process fully enclosed: No Effective housekeeping practices in place: Yes Work area: Outdoors Source located close to buildings: Yes Primary localized controls: no (0.00 % reduction) Secondary localized control: no (0.00 % reduction) The predicted air concentration (90th percentile) in a worker's personal breathing zone outside of any Respiratory Protection Equipment (RPE) is 0.008 mg/m^3.

10. RISK CHARACTERISATION

The scenarios described in chapter 9 ff result in an exposure of environment, workers and consumers. In order to determine if this specific exposure is safe for a specific scenario, the exposure is put into relation to the corresponding indicative reference value (e.g. DNEL, PNEC). The resulting risk characterisation ratio (RCR) indicates if the specific scenario is safe or not. In addition to individual exposure estimates also exposure from combined routes and compartments are displayed, as well as combined exposure from different scenarios.

10.1 Scenario 1: Solvent for Production of a Fine Chemical

The following RCR calculations refer to the contributing scenarios described in chapter 9.1

10.1.1 Contributing Scenario (1) controlling environmental exposure for ERC7

Solvent for Production of a Fine Chemical

The quantitative risk characterisation for this environmental exposure has been calculated using EasyTRA.

The environmental exposure calculation per compartment is based on the algorithms of the EU TGD 2003 Risk Assessment Spreadsheet Model 1.24a.

10.1.1.1 Aquatic compartment (including sediment)

Table 5. Environmental risk aquatic of ES 1.1

Compartments	PEC	PNEC	RCR = PEC/PNEC	MSafe kg/d
Freshwater	0.000386 mg/L	6.4 mg/L	0.00006	1.66E8
Freshwater sediment	0.001413 mg/kg_{dwt}	27.4 mg/kg_{dwt}	0.000052	1.94E8
Marine water	0.000583 mg/L	0.640 mg/L	0.000912	1.10E7
Marine water sediment	0.002138 mg/kg_{dwt}	2.74 mg/kg_{dwt}	0.00078	1.28E7

10.1.1.2 Terrestrial compartment

Table 6. Environmental risk terrestrial of ES 1.1

Compartments	PEC	PNEC	RCR = PEC/PNEC	MSafe kg/d
Agricultural soil	0.002911 mg/kg_{dwt}	1.72 mg/kg_{dwt}	0.001693	5.91E6

10.1.1.3 Microbiological activity in sewage treatment systems

Table 7. Environmental risk STP of ES 1.1

Compartments	PEC	PNEC	RCR = PEC/PNEC	MSafe kg/d
STP	0.055 mg/L	50 mg/L	0.0011	9.09E6

10.1.1.4 Man via environment

Secondary poisoning considers indirect exposure of man via foods, air and drinking water. The following table shows the calculated exposure to the substance from exemplary food sources at different trophic levels together with the total exposure over all routes and food sources.

Table 8. Environmental risk man via environment of ES 1.1

Food source	Exposure concentration (EC)	DNEL	Risk characterisation ratio = EC/DNEL	MSafe kg/d
Fish	7.66E-7 mg/kg_{bw}/day	1.04 mg/kg_{bw}/day	7.36E-7	-
Root crop	6.56E-6 mg/kg_{bw}/day	1.04 mg/kg_{bw}/day	6.30E-6	-
Leaf crop	5.79E-6 mg/kg_{bw}/day	1.04 mg/kg_{bw}/day	5.56E-6	-
Milk	5.93E-9 mg/kg_{bw}/day	1.04 mg/kg_{bw}/day	5.70E-9	-
Meat	3.18E-10	1.04	3.06E-10	-

Food source	Exposure concentration (EC)	DNEL	Risk characterisation ratio = EC/DNEL	MSafe kg/d
	mg/kg$_{bw}$/day	mg/kg$_{bw}$/day		
Drinking water	0.000037 mg/kg$_{bw}$/day	1.04 mg/kg$_{bw}$/day	0.000035	-
inhalation	8.80E-8 mg/kg$_{bw}$/day	1.04 mg/kg$_{bw}$/day	8.46E-8	-
Total	0.00005 mg/kg$_{bw}$/day	1.04 mg/kg$_{bw}$/day	0.000048	2.09E8

10.1.1.5 Secondary poisoning

Table 9. Environmental risk secondary poisoning of ES 1.1

Food source	Exposure concentration (EC)	PNECoral	RCR = PEC/PNEC	MSafe kg/d
Fish	0.000468 mg/kg food	2.77 mg/kg food	0.000169	-
Fish, marine	0.000068 mg/kg food	2.77 mg/kg food	0.000025	-
Fish predator, marine	0.000051 mg/kg food	2.77 mg/kg food	0.000019	-
Worm	0.008183 mg/kg food	2.77 mg/kg food	0.002954	-
Total	0.008183 mg/kg$_{bw}$/day	2.77 mg/kg$_{bw}$/day	0.002954	3.39E6

10.1.2 Contributing Scenario (2) controlling industrial worker exposure for PROC 8B

Solvent for Production of a Fine Chemical - Diglyme charging into Fine Chemical synthesis at

production site

The quantitative risk characterisation for this worker exposure has been calculated by EasyTRA.

The following table shows the exposure estimations via the dermal and inhalation route together with the total exposure of workers over all routes if applicable.

Table 10. Worker risk of ES 1.2

Route	Exposure concentration (EC)	DNEL	Risk characterisation ratio = EC/DNEL
dermal, long-term systemic	0.120 mg/kg_{bw}/day	0.240 mg/kg_{bw}/day	0.500
inhalation, long-term systemic	0.003 mg/m^3	1.68 mg/m^3	0.001786
Combined routes	0.120429 mg/kg_{bw}/day	-	0.501786

10.1.3 Contributing Scenario (3) controlling industrial worker exposure for PROC 1

Solvent for Production of a Fine Chemical - Synthesis of a fine chemical

The quantitative risk characterisation for this worker exposure has been calculated by EasyTRA.

The following table shows the exposure estimations via the dermal and inhalation route together with the total exposure of workers over all routes if applicable.

Table 11. Worker risk of ES 1.3

Route	Exposure concentration (EC)	DNEL	Risk characterisation ratio = EC/DNEL
dermal, long-term systemic	0.034286 mg/kg_{bw}/day	0.240 mg/kg_{bw}/day	0.142857
inhalation, long-term systemic	0.055908 mg/m^3	1.68 mg/m^3	0.033279
Combined routes	0.042273 mg/kg_{bw}/day	-	0.176136

10.1.4 Contributing Scenario (4) controlling industrial worker exposure for PROC 9

Solvent for Production of a Fine Chemical - Sample taking of fine chemical and transport to quality laboratory

The quantitative risk characterisation for this worker exposure has been calculated by EasyTRA.

The following table shows the exposure estimations via the dermal and inhalation route together with the total exposure of workers over all routes if applicable.

Table 12. Worker risk of ES 1.4

Route	Exposure concentration (EC)	DNEL	Risk characterisation ratio = EC/DNEL
dermal, long-term systemic	1.00E-6 mg/kg_{bw}/day	0.240 mg/kg_{bw}/day	4.17E-6
inhalation, long-term systemic	0.021 mg/m^3	1.68 mg/m^3	0.0125
Combined routes	0.003001 mg/kg_{bw}/day	-	0.012504

10.1.5 Contributing Scenario (5) controlling industrial worker exposure for PROC 15

Solvent for Production of a Fine Chemical - Handling at quality control laboratory

The quantitative risk characterisation for this worker exposure has been calculated by EasyTRA.

The following table shows the exposure estimations via the dermal and inhalation route together with the total exposure of workers over all routes if applicable.

Table 13. Worker risk of ES 1.5

Route	Exposure concentration (EC)	DNEL	Risk characterisation ratio = EC/DNEL

Route	Exposure concentration (EC)	DNEL	Risk characterisation ratio = EC/DNEL
dermal, long-term systemic	0.002057 $mg/kg_{bw}/day$	0.240 $mg/kg_{bw}/day$	0.008571
inhalation, long-term systemic	0.0012 mg/m^3	1.68 mg/m^3	0.000714
Combined routes	0.002229 $mg/kg_{bw}/day$	-	0.009286

10.1.6 Contributing Scenario (6) controlling industrial worker exposure for PROC 8B

Solvent for Production of a Fine Chemical - Product isolation in a dedicated filter press

The quantitative risk characterisation for this worker exposure has been calculated by EasyTRA.

The following table shows the exposure estimations via the dermal and inhalation route together with the total exposure of workers over all routes if applicable.

Table 14. Worker risk of ES 1.6

Route	Exposure concentration (EC)	DNEL	Risk characterisation ratio = EC/DNEL
dermal, long-term systemic	0.082286 $mg/kg_{bw}/day$	0.240 $mg/kg_{bw}/day$	0.342857
inhalation, long-term systemic	0.130 mg/m^3	1.68 mg/m^3	0.077381
Combined routes	0.100857 $mg/kg_{bw}/day$	-	0.420238

10.1.7 Contributing Scenario (7) controlling industrial worker exposure for PROC 8B

Solvent for Production of a Fine Chemical - Final Product Transfer from the drying chamber into small container

The quantitative risk characterisation for this worker exposure has been calculated by EasyTRA.

The following table shows the exposure estimations via the dermal and inhalation route together with the total exposure of workers over all routes if applicable.

Table 15. Worker risk of ES 1.7

Route	Exposure concentration (EC)	DNEL	Risk characterisation ratio = EC/DNEL
dermal, long-term systemic	0.0012 mg/kg_{bw}/day	0.240 mg/kg_{bw}/day	0.005
inhalation, long-term systemic	0.0001 mg/m^3	1.68 mg/m^3	0.00006
Combined routes	0.001214 mg/kg_{bw}/day	-	0.00506

10.1.8 Contributing Scenario (8) controlling industrial worker exposure for PROC 9

Solvent for Production of a Fine Chemical - Analytical sampling (Diglyme content control in wash water) from waste storage tank [redacted]

The quantitative risk characterisation for this worker exposure has been calculated by EasyTRA.

The following table shows the exposure estimations via the dermal and inhalation route together with the total exposure of workers over all routes if applicable.

Table 16. Worker risk of ES 1.8

Route	Exposure concentration (EC)	DNEL	Risk characterisation ratio = EC/DNEL
dermal, long-term systemic	0.0002 mg/kg_{bw}/day	0.240 mg/kg_{bw}/day	0.000833
inhalation, long-term systemic	0.0016 mg/m^3	1.68 mg/m^3	0.000952
Combined routes	0.000429 mg/kg_{bw}/day	-	0.001786

10.1.9 Contributing Scenario (9) controlling industrial worker exposure for PROC 8B

Solvent for Production of a Fine Chemical - Partial waste transfer to road tanker

The quantitative risk characterisation for this worker exposure has been calculated by EasyTRA.

The following table shows the exposure estimations via the dermal and inhalation route together with the total exposure of workers over all routes if applicable.

Table 17. Worker risk of ES 1.9

Route	Exposure concentration (EC)	DNEL	Risk characterisation ratio = EC/DNEL
dermal, long-term systemic	0.0009 mg/kg_{bw}/day	0.240 mg/kg_{bw}/day	0.00375
inhalation, long-term systemic	0.008 mg/m^3	1.68 mg/m^3	0.004762
Combined routes	0.002043 mg/kg_{bw}/day	-	0.008512

10.2 Overall exposure (combined for all relevant emission/release sources)

10.2.1 Local release of all wide dispersive uses (including regional exposure)

The regional exposure represents the steady-state concentration of a given substance in the environmental compartments after all partitioning and degradation processes have been taken into account. In addition the aggregated emissions from all wide dispersive uses at a local STP are considered as well. From the calculated predicted environmental concentrations (PECs) and the corresponding predicted no-effect concentrations (PNECs) risk characterization ratios (RCRs) for the standard region are derived the same way as for the local scale. The calculations of the regional PECs were performed utilizing the SimpleBox Model as proposed by the TGD, local emissions at the STP were calculated using the formulae given in the TGD.

10.2.1.1 Aquatic compartment (including sediment)

Table 18. Aquatic compartment (including sediment)

Compartments	PEC	PNEC	RCR = PEC/PNEC
Freshwater	0.000331 mg/L	6.4 mg/L	0.000052
Freshwater sediment	0.000228 mg/kg_{dwt}	27.4 mg/kg_{dwt}	8.34E-6
Marine water	0.000033 mg/L	0.640 mg/L	0.000052
Marine water sediment	0.000023 mg/kg_{dwt}	2.74 mg/kg_{dwt}	8.56E-6

10.2.1.2 Terrestrial compartment

Table 19. Terrestrial compartment

Compartments	PEC	PNEC	RCR = PEC/PNEC
Agricultural soil	0.000042 mg/kg_{dwt}	1.72 mg/kg_{dwt}	0.000025
Grassland	0.000042 mg/kg_{dwt}	1.72 mg/kg_{dwt}	0.000025

10.2.3.1 Total releases

Table 20. Total releases

Release route	Total releases per year
water	10 to/year
air	10 to/year
soil	10 to/year