SDS EXPOSURE SCENARIO (ES)
AMMONIA (ANHYDROUS)

Annex 1: Exposure Scenario (ES)

Exposure assessment

Anhydrous and aqueous ammonia are extensively used across a broad range of industrial, professional and domestic applications. Ammonia in the anhydrous form is one of the most highly produced inorganic chemicals. Anhydrous ammonia is a gaseous substance at room temperature at 20°C. During the life-cycle of anhydrous ammonia, the substance may be diluted with water to produce the aqueous form of ammonia, typically at concentrations up to 25% w/w.

In this section, an assessment of the potential exposures associated with industrial, professional and consumer uses of anhydrous and aqueous forms of ammonia has been carried out. Since the uses of ammonia are extensive and broad, it is beyond the scope of this report to present a detailed assessment of exposure for all possible use scenarios. An exposure assessment has therefore been carried out for six generic Exposure Scenarios: ES 1 – Manufacturing of anhydrous ammonia, ES 2 – Distribution and formulation of anhydrous ammonia, ES3 – Industrial uses of anhydrous ammonia as an intermediate, ES 4 - Industrial end-use of anhydrous and aqueous ammonia (processing, non-processing aids, auxiliary agent), ES 5 – Wide dispersive end-use: Professional uses of anhydrous and aqueous ammonia ES 6 – Wide dispersive end-use: Consumer uses of aqueous ammonia. To ensure that the uses of ammonia are addressed as comprehensively as possible in this exposure assessment, for each exposure scenario, exposures have been determined for a range of operational conditions, taking into account the impact of different risk management measures.

Table 1 gives a summary of the exposure scenarios addressed in this section.

SDS EXPOSURE SCENARIO (ES)

AMMONIA (ANHYDROUS)

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

ES number	Volume (tonnes)	Manufacture	Identified uses			Resulting life cycle stage		Linked to Identified Use	Sector of Use (SU)	Preparation Category (PC)	Process category (PROC)	ERC
			Formulation	Industrial and/or wide dispersive use	Consumer use	Service life (for articles)	Waste stage					
ES 1: Manufacturing of anhydrous ammonia		X							SU8, SU9, C20.1.5		PROC 1, 2, 8a, 8b	ERC 1
ES 2: Distribution and formulation of anhydrous ammonia			X						SU1, SU10, SU24		PROC 1, 2, 3, 4, 5 8a, 8b, 9, 15	ERC2
ES 3: Industrial uses of anhydrous ammonia as an intermediate			X	X					SU1, SU5, SU8, SU9, SU12, SU15, SU24, C21, C20.1.5		PROC 1, 2, 3, 4, 5, 8a, 8b, 9, 15	ERC 6a
ES 4: Industrial end-use of anhydrous and aqueous ammonia (processing, non-processing aids, auxiliary agent				X					SU4, SU5, SU6a, SU6b, SU7, SU8, SU11, SU12, SU13, SU15, SU16, SU 23, NACE C28.2.5		PROC 1, 2, 3, 4, 5, 7, 8a, 8b, 9, 10, 13,15,19	ERC 4, 5, 6b, 7
ES 5: Wide dispersive end-use :Professional uses of anhydrous and aqueous ammonia				X					SU1, SU10, SU23		PROC 1, 2, 3, 4, 5, 8a, 8b, 9, 10, 11, 13, 15, 18, 19	ERC 8a, 8b, 8d, 8e, 8f, 9a, 9b, 11a
ES 6: Wide dispersive end-use: Consumer uses of aqueous ammonia					X	X				PC9a, PC9b, PC9c, PC1, PC12, PC16, PC18, PC20, PC23, PC35, PC37, PC39 UCN CODE A40200		ERC 8a, 8b, 8d, 8e, 8f, 9a, 9b, 11a

1.1 Exposure Scenario 1: Manufacturing of anhydrous ammonia

1.1.1 Exposure scenario

Ammonia, in the anhydrous form, is one of the most highly produced inorganic chemicals due to its broad and diverse range of uses. Ammonia manufacturing facilities provide the base anhydrous liquid which is formulated into aqueous solutions of ammonia, used as an intermediate in the chemical industry or within a range of industrial sectors as a processing agent or reagent and incorporated into products intended for use by professionals and consumers. Dozens of large-scale chemical plants worldwide produce ammonia, some of which produce as much as 2000 to 3000 tonnes of anhydrous ammonia in liquid form per day.

Anhydrous ammonia (>99.5 % wt) is manufactured by high temperature and pressure synthesis in large facilities. A typical ammonia-producing industrial plant first coverts natural gas (e.g. methane), liquefied petroleum gas (e.g. propane and butane) or petroleum naphtha into gaseous hydrogen. The method for producing hydrogen from hydrocarbons is referred to as "steam reforming". Several processes are involved in producing hydrogen from a natural gas feedstock including sulphur and carbon dioxide removal and methanation to remove any small residual amounts of carbon dioxide or carbon monoxide. Catalytic shift conversion is used to convert CO to CO_2 and hydrogen. Hydrogen is then catalytically reacted with nitrogen (derived from air) in the ratio 3:1 by volume and compressed to around 200 times atmospheric pressure (up to 1000 atm or 100 megapascals) at high temperatures of around 700°C to form anhydrous liquid ammonia. This step is known as the ammonia synthesis loop (e.g. the Haber-Bosch process).

Steam reforming, shift conversion, carbon dioxide removal, methanation and the Haber-Bosch process are carried out at absolute pressures ranging from 25 to 35 bar depending on the design of the ammonia synthesis plant.

1.1.1.1 Description of activities and processes covered in the exposure scenario

Due to the large size of facilities that manufacture anhydrous ammonia, vessels and reactors for gas synthesis and processing are housed outdoors. Other processes may be carried out indoors, e.g. compression of synthesis gas in compression units. Processes are continuous and are carried out in closed pipelines and vessels.

During the manufacturing of anhydrous ammonia, operators monitor and control processes across a number of units: gas compression, methanation, synthesis loop, ammonia cooling units and storage. Most manufacturing processes and plant are operated automatically by a small number of operators located in separate control rooms. Operators may also carry out routine 'field' inspections around the facility to check that equipment is operating correctly. Other manual operations in the field may also be undertaken such as: preparation of equipment for mechanical or other work (e.g. maintenance), or taking samples or measurements. Operators load ammonia stored in spheres onto tankers for distribution by rail or road. Tanker loading generally takes place in the open air and involves opening and closing valves and connecting and disconnecting pipes and hoses.

1.1.1.2 Operational conditions related to frequency and duration

Anhydrous ammonia is manufactured by closed, continuous processes which can run for long periods without interruption, for up to 24 hours/day, 330-360 days per year. Operational control and some field activities such as inspection tours are therefore also carried out continuously (e.g. in shifts covering 24 hour periods daily, without interruption of the processes). Although operators generally work standard shifts of 8 hours/day and a normal working week, with production continuing at weekends, longer shifts up to 12 hours /day can also be carried out. Operators will typically work for 220 days/year. During a typical shift, operators may spend 80 % of their time in a control room and 20 % of their time in the field. Duration of typical field operations can be 120-240, 30 and 60 minutes respectively for inspection tours, sampling and measuring and preparation work. Several inspection tours may be carried out during one shift. Tanker loading is also carried out daily. Other activities may be more intermittent: maintenance work and sampling may be carried out on 20 and 12 days per year respectively.

1.1.1.3 Risk management measures

The manufacturing of anhydrous ammonia involves special equipment and high integrity contained systems with little or no potential for worker exposure. These facilities are usually housed outdoors, with workers being segregated in separate control rooms with no direct contact with manufacturing units. The likelihood of industrial workers being exposed to ammonia when controlling manufacturing processes is therefore low, since these workers are located in separate control rooms.

Workers may potentially be exposed to ammonia when conducting field activities (e.g. when operating valves, pumps or tanks etc). All operations are performed in a closed system. Pipelines and vessels are sealed and insulated and sampling is carried out with a closed sample loop. Extract ventilation is provided at openings and points were emission may occur. Anhydrous ammonia is stored in closed containers and tanks and is transferred under containment. A good standard of general or controlled ventilation is applied when maintenance activities are carried out. Personal protective clothing (e.g. face/eye protection, helmet, gloves, boots and protective overalls) is worn when any potential contact may arise.

All technological devices have a proper quality certification, and are regularly controlled and maintained to avoid the uncontrolled discharge of ammonia.

Good occupational hygiene and exposure control measures are implemented to minimise the potential for worker exposure. Workers involved in the manufacture, sampling and transfer of anhydrous ammonia to road tankers are well-trained in these procedures and use of appropriate protective equipment.

1.1.2 Exposure estimation

The assessment of worker exposure to anhydrous ammonia during manufacturing (ES 1) was carried out for processes relevant to this scenario as identified by PROC codes reflecting: use and storage of ammonia in closed systems with no likelihood of exposure (PROC 1), use in closed, continuous processes with occasional controlled exposure (PROC 2), maintenance and clean-down (PROC 8a) and transfer (PROC 8b). A screening-level (Tier 1) assessment of worker exposure was carried out using the ECETOC Targeted Risk Assessment (TRA) model. The ECETOC TRA was used to predict dermal exposures (expressed as a daily systemic dose in mg/kg bw) and inhalation exposure concentrations (expressed as an airborne concentrations in mg/m^3) associated with each process defined by PROC codes.

Exposure to workers was assessed taking into account different operational conditions that may be associated with the manufacturing of anhydrous ammonia and the impact of different exposure control measures. Exposures were determined for task durations of 1- 4 hours or >4 hours and assuming that process are carried out either outdoors, indoors without use of local exhaust ventilation (LEV) or indoors with the use of LEV. To reflect the use of personal protective equipment (PPE), dermal exposures were determined assuming either no gloves or gloves affording 90 % protection of the hands are worn. To reflect the use of respiratory protective equipment (RPE), inhalation exposure concentrations were determined assuming either no RPE or RPE affording 95% protection is worn.

Parameters used in the ECETOC TRA model are: molecular weight (17 $g.mol^{-1}$ for anhydrous ammonia) and vapour pressure (8.6 x 10^5 Pa at 20°C for anhydrous ammonia). Systemic dermal exposures have been determined for a worker with bodyweight 70 kg.

1.1.2.1 Workers exposure

1.1.2.1.1 Acute/Short term and long-term exposure

Potential systemic dermal exposures and inhalation exposure concentrations predicted by the ECETOC TRA model for processes associated with the manufacturing of anhydrous ammonia are shown in Tables 2 and 3 respectively. ECETOC predicts a daily systemic dose following dermal exposure and a typical daily inhalation exposure concentration and does not specifically predict acute (short-term) and chronic (long-term) exposures. In the risk characterisation, dermal and inhalation exposures predicted by ECETOC are compared with acute and chronic DNEL values for local and systemic effects to determine the potential risk to human health associated with ES 1.

Table 2: Dermal exposures to anhydrous ammonia predicted using the ECETOC TRA model for industrial workers during manufacturing (ES 1).

Description of activity	PROC	Exposure assumptions		Estimated Exposure mg/kg bw/d	
		Duration	Use of ventilation	No gloves worn	Gloves worn (90% reduction)
Use in a closed process, no likelihood of exposure: storage (closed or bulk container)	PROC 1	1-4 hrs or >4 hrs	Outdoors /Indoors without LEV	0.34	0.03
Use in a closed, continuous process with occasional controlled exposure (e.g. sampling)	PROC 2	1-4 hrs or >4 hrs	Outdoors /Indoors without LEV	1.37	0.14
			Indoors with LEV	0.14	0.01
Maintenance, clean down	PROC 8a	1-4 hrs or >4 hrs	Outdoors / Indoors without LEV	13.71	1.37
			Indoors with LEV	0.14	0.01
Transfer (charging/discharging) from or to vessels or large containers at dedicated facilities	PROC 8b	1-4 hrs or >4 hrs	Outdoors / Indoors without LEV	6.86	0.69
			Indoors with LEV	0.69	0.07

Table 3: Inhalation exposure concentrations for anhydrous ammonia predicted using the ECETOC TRA model for industrial workers during manufacturing (ES 1)

Description of activity	PROC	Exposure assumptions		Estimated Inhalation Exposure Concentration mg/m^3	
		Duration	Use of ventilation	No RPE	RPE (95% reduction)
Use in a closed process, no likelihood of exposure: Storage (closed bulk or container)	PROC 1	1-4 hrs or >4 hrs	Outdoors	0.00	NA
			Indoors without LEV	0.01	NA
Use in a closed, continuous process with occasional controlled exposure (e.g. sampling)	PROC 2	>4hrs	Outdoors	24.79	1.24
			Indoors without LEV	35.42	1.77
			Indoors with LEV	3.54	0.18
		1-4 hrs	Outdoors	14.88	0.74
			Indoors without LEV	22.25	1.06
			Indoors with LEV	2.13	0.11

Maintenance, clean down	PROC 8a	>4hrs	Outdoors	123.96	6.20
			Indoors without LEV	177.08	8.85
			Indoors with LEV	17.71	0.89
		1-4 hrs	Outdoors	74.38	3.72
			Indoors without LEV	106.25	5.31
			Indoors with LEV	10.63	0.53
Transfer (charging/discharging) from/to vessels or large containers at dedicated facilities	PROC 8b	>4hrs	Outdoors	74.38	3.72
			Indoors without LEV	106.25	5.31
			Indoors with LEV	3.19	0.16
		1-4 hrs	Outdoors	44.63	2.23
			Indoors without LEV	63.75	3.19
			Indoors with LEV	1.91	0.10

1.1.2.2 General public / consumer exposure

Manufacturing of anhydrous ammonia is carried out at industrial sites from which members of the public are excluded. Members of the public will not therefore be exposed to anhydrous ammonia during manufacturing processes. Consumer exposures to ammonia in the diluted (aqueous) form have been assessed in Section 1.6; ES 6.

1.1.2.3 Indirect exposure of humans via the environment (oral)

Ammonia is ubiquitous in the environment with <30% of emissions resulting from fertiliser uses and from non-agricultural sources (ref. 'Ammonia in the UK' - DEFRA).

In addition, there is no evidence that ammonia bioaccumulates as the log Kow value is 0.23. Since the trigger of BCF >100 (log Kow>3) is not met, the derivation of PNECs to protect against secondary poisoning is not required.

The risk of indirect exposure of humans via the environment is therefore not considered

1.1.2.4 Environmental exposure

First tier conservative environmental exposure estimations were carried out using EUSES 2.1 and with the specified defaults.

Second tier worst case environmental exposure estimations were carried out using EUSES 2.1 to take into account more realistic factors that affect the environmental concentrations.

1.1.2.4.1 Environmental releases

The environmental releases are determined primarily by tonnage and the ERC in the first tier with conservative estimations and defaults being implemented in EUSES. For the second tier assessments in EUSES, more realistic inputs were chosen to best suit the description of the production and uses of anhydrous ammonia. Emission defaults are those specified by the ECHA "Guidance on information requirements and chemical safety assessment: Chapter R.16: Environmental Exposure Estimation". Regional data and emission fractions were calculated using EUSES. Full EUSES inputs are shown below.

Table 4: EUSES inputs for environmental assessment

Input parameter:	Value:	Unit:	ERC default (if applicable)
Molecular Weight	35	g/mol	Value for aqueous ammonia used as it is this form which will predominate in the environment.
Vapour Pressure (at 20 °C)	287	hPa	Value for aqueous ammonia used as it is this form which will predominate in the environment.
Water Solubility	4.82×10^5	mg/L	
Octanol/water partition coefficient	0.23	logKow	
Koc	13.8	L/kg	Modelled output used based on default 'non-hydrophobics' QSAR class within EUSES.
Biodegradability	Readily biodegradable		
Life Cycle Step	Industrial use		
Environmental Release Class	ERC 1		
Fraction of Tonnage for Region			1
STP			Yes
Emission events per year	330	Days	Based on worst case emission events supplied by consortium members.
Default Release to Air for ERC 1	5	%	5
Default Release to Water for ERC 1	6	%	6
Dilution factor applied for PEC derivation	10		10 (20,000 m^3/d)
Tonnage assessed	Total: 6,591,429 Regional: 950,000	tonnes/annum	Of 20 companies, 7 responded with tonnage data. The total of 2,307,000 tonnes was normalized by a factor representing the number of companies in each use to estimate the total tonnage across the industry. Regional tonnage was taken to be the largest individual reported volume.

Table 5 Predicted Releases to the Environment Tier 1

ERC	Compartments	Predicted releases	Measured release	Explanation / source of measured data
1	Release to air	1.44×10^5 kg/day	-	Predicted values are those calculated by EUSES using the tonnage data and defaults for ERC1.
	Release to wastewater	1.73×10^5 kg/day	-	Predicted values are those calculated by EUSES using the tonnage data and defaults for ERC1.
	Soil (direct only) Agricultural soil	0	-	No direct loss to soil is expected for this ERC.

**The predicted releases were estimated using the EUSES 2.1 program.*

In reality removal of ammonia in sewage treatment plants is highly efficient being removed first by nitrification to nitrate followed by denitrification resulting in the release of nitrogen gas. Complete consumption within the STP can be assumed and this has been used in the tier 2 assessment within EUSES.

Table 6: Measured values for tier 2 assessment.

scription of RMM	Details	Effect taken into account in EUSES	Comments
Efficient removal of ammonia in STP.	0 mg/L (Local) 0 kg/d (Regional)	Lowering of calculated concentration in STP effluent. Applied at both a local and a regional level. All regional emissions to STP.	

Table 7 Predicted Releases to the Environment Tier 2

ERC	Compartments	Predicted releases	Measured release	Explanation / source of measured data
1	Release to air	1.44×10^5 kg/day	-	Predicted values are those calculated by EUSES using the tonnage data and defaults for ERC1.
	Release to wastewater	1.73×10^5 kg/day	-	Predicted values are those calculated by EUSES using the tonnage data and defaults for ERC1.
	Soil (direct only) Agricultural soil	0	-	No direct loss to soil is expected for this ERC

1.1.2.4.2 Exposure concentration in sewage treatment plants (STP)

Table 8: Tier 1 Concentrations in sewage

ERC for Compartment:	Estimated exposure concentrations		Measured exposure concentrations		Explanation / source of measured data
	value	unit	value	unit	
Waste water before treatment	8.63×10^4	mg/L	NA	mg/L	
Sewage (STP effluent)	1.07×10^4	mg/L	NA	mg/L	
Local freshwater	1070	mg/L	NA	mg/L	10-fold dilution by receiving waters. Local concentration with atmospheric deposition not yet taken into account.

Table 9: Tier 2 Concentrations in sewage

ERC for Compartment:	Estimated exposure concentrations		Measured exposure concentrations		Explanation / source of measured data
	Value	unit	value	unit	
Waste water before treatment	8.63×10^4	mg/L	NA	mg/L	
Sewage (STP effluent)	0	mg/L	NA	mg/L	Based on efficient removal by STP
Local freshwater	0	mg/L	NA	mg/L	10-fold dilution by receiving waters. Local concentration with atmospheric deposition not yet taken into account.

Table 10: General emission fractions from the municipal STP

Fraction description	Fraction amount	
	value	unit
Fraction of emission directed to air by STP	0.583	%
Fraction of emission directed to water by STP	12.4	%
Fraction of emission directed to sludge by STP	0.13	%
Fraction of emission degraded by STP	86.8	%

1.1.2.4.3 Exposure concentration in aquatic compartment

Table 11: Tier 1 Local concentrations in aquatic compartment

Compartments	Local concentration aquatic (local mg/L)	Justification
ERC1 Freshwater (in mg/L)	1070	
ERC1 Marine water (in mg/L)	107	10-fold dilution by receiving waters

Table 12: Tier 1 Predicted Environmental Concentrations (PEC) in aquatic compartment

Compartments	PEC aquatic (local mg/L)	Justification
ERC1Freshwater (in mg/L)	1070	
ERC1 Marine water (in mg/L)	107	10-fold dilution by receiving waters

Table 13: Tier 2 Local concentrations in aquatic compartment

Compartments	Local concentration aquatic (local mg/L)	Justification
Freshwater (in mg/L)	0	
Marine water (in mg/L)	0	10-fold dilution by receiving waters
Intermittent releases to water (in mg/L)	NA	Intermittent release not relevant

Table 14: Tier 2 Predicted Environmental Concentrations (PEC) in aquatic compartment

Compartments	PEC aquatic (local mg/L)	Justification
Freshwater (in mg/L)	3.48×10^{-3}	
Marine water (in mg/L)	7.61×10^{-4}	
Intermittent releases to water (in mg/L)	NA	Intermittent release not relevant

1.1.2.4.4 Exposure concentration in sediments

Table 15: Tier 1 Predicted Environmental Concentrations (PEC) in aquatic sediment compartment

Compartments	PEC aquatic (local)
ERC1 Freshwater sediment (in mg/kg)	1160
ERC1 Marine sediment (in mg/kg)	116

Table 16: Tier 2 Predicted Environmental Concentrations (PEC) in aquatic sediment compartment

Compartments	PEC aquatic (local)
Freshwater sediment (in mg/kg)	3.76×10^{-3}
Marine sediment (in mg/kg)	8.24×10^{-4}

1.1.2.4.5 Exposure concentrations in soil and groundwater

Upon contact with soil, ammonia will be rapidly converted by a variety of bacteria, actinomycetes and fungi to ammonium (NH_4^+) by the process of ammonification or mineralization. Ammonium is then rapidly converted to nitrate. Nitrate is subsequently taken up and utilised by plants or returned to the atmosphere following denitrification; the metabolic reduction of nitrate into nitrogen or nitrous oxide (N20) gas. The most likely fate of ammonium ions in soils is conversion to nitrates by nitrification. Therefore accumulation of concentrations of ammonia in soil and groundwater will not be expected.

1.1.2.4.6 Atmospheric compartment

Table 17: Tier 1 local concentrations in air

ERC		Estimated local exposure concentrations	Explanation / source of data
1	During emission (mg/m3)	40	Estimated using EUSES 2.1
	Annual average (mg/m3)	36.1	Estimated using EUSES 2.1
	Annual deposition (mg/m²/d)	52.4	Estimated using EUSES 2.1

Table 18: Tier 1 Predicted Exposure Concentration (PEC) in air

ERC		Local concentration	PEC air (local+regional)	Justification
1	Annual average PEC in air, total (mg/m3)	36.1	36.1	Estimated using EUSES 2.1.

Table 19: Tier 2 local concentrations in air

ERC		Estimated local exposure concentrations	Explanation / source of data
1	During emission (mg/m3)	40	Estimated using EUSES 2.1
	Annual average (mg/m3)	36.1	Estimated using EUSES 2.1
	Annual deposition (mg/m²/d)	52.4	Estimated using EUSES 2.1

Table 20: Tier 2 Predicted Exposure Concentration (PEC) in air

ERC		Local concentration	PEC air (local+regional)	Justification
1	Annual average PEC in air, total (mg/m3)	36.1	36.1	Estimated using EUSES 2.1.

1.1.2.4.7 Exposure concentration relevant for the food chain (Secondary poisoning)

In terms of secondary poisoning, there is no evidence that ammonia bioaccumulates as the log Kow value is 0.23. Since the trigger of BCF >100 (log Kow>3) is not met, the derivation of PNECs to protect against secondary poisoning is not required. Risk characterisation ratios cannot therefore be derived.

1.1.2.4.8 Regional exposure levels and environmental concentrations

Anhydrous ammonia is produced and used at many sites throughout a region and this may lead to a degree of regional exposure. Regional exposure has been modelled for this exposure scenario using the regional module of EUSES 2.1.

Table 21: Tier 1 Regional concentrations in the environment

	Predicted regional Exposure Concentrations		Measured regional exposure concentrations		Explanation / source of measured data
	PEC value	unit	Measured value	unit	
Freshwater	0.0913	mg/L	NA	mg/L	
Marine water	0.00836	mg/L	NA	mg/L	
Freshwater sediments	0.0869	mg/kg	NA	mg/kg	
Marine sediments	0.00802	mg/kg	NA	mg/kg	
Agricultural soil	0.00170	mg/kg	NA	mg/kg	
Grassland	0.00208	mg/kg	NA	mg/kg	
Air	0.00316	mg/m^3	NA	mg/m^3	

Table 22: Tier 2 Regional concentrations in the environment

	Predicted regional Exposure Concentrations		Measured regional exposure concentrations		Explanation / source of measured data
	PEC value	unit	Measured value	unit	
Freshwater	3.48×10^{-3}	mg/L	NA	mg/L	
Marine water	7.71×10^{-4}	mg/L	NA	mg/L	
Freshwater sediments	3.31×10^{-3}	mg/kg	NA	mg/kg	
Marine sediments	7.30×10^{-4}	mg/kg	NA	mg/kg	
Agricultural soil	1.64×10^{-3}	mg/kg	NA	mg/kg	
Grassland	1.79×10^{-3}	mg/kg	NA	mg/kg	
Air	2.73×10^{-3}	mg/m^3	NA	mg/m^3	

1.2 Exposure Scenario 2: Distribution and formulation of anhydrous ammonia

1.2.1 Exposure scenario

Manufactured anhydrous liquid ammonia (>99.5 % wt) is distributed widely to many industrial and municipality users. Anhydrous liquid ammonia is transported to chemical formulation facilities which produce aqueous solutions of ammonia. Aqueous ammonia products are then distributed to a wide range of industrial end-users and is also used to produce products for professional and consumer users.

1.2.1.1 Description of activities and processes covered in the exposure scenario

Manufactured anhydrous liquid ammonia is stored and transported as a liquid under pressure by rail, road or water in specialised, authorised containers (e.g. tanks and tank trucks approved for transporting ammonia). When transported in tanks, the pressure on the tank is the liquid pressure and remains the same whether the tank is 10% or 80% full. The maximum filling level of an anhydrous ammonia tank is 85%. Anhydrous liquid ammonia may also be distributed to end-user industries via pipeline systems.

Anhydrous liquid ammonia is used to produce aqueous ammonia solutions (5-25% w/w). The anhydrous liquid ammonia product is transported to chemical manufacturing facilities by rail or road where it is blended with deionised water to produce solutions of aqueous ammonia that are used for a broad range of applications. Aqueous ammonia solution products are distributed to a wide range of industrial users by road or rail in various quantities (e.g. tanks or 1, 5, 15 and 50 gallon containers). Distributors of anhydrous and aqueous ammonia can operate on a regional or national level.

1.2.1.2 Operational conditions related to frequency and duration

Distribution and formulation of ammonia is carried out by continuous or batch processes indoors and outdoors in closed systems. Processes involve storage, charging, loading, transfer and filling containers.

Workers involved in the distribution of anhydrous ammonia load tanks and containers on various transportation vehicles including barges, trains or road tankers. Loading rail tank or road tankers may typically be carried out for between 100 minutes to 8 hours/day, up to 2 times a week. Loading of a train can take up to 20 hours. Smaller tanks or containers can be loaded in 15 minutes, 1-2 times per shift, 2-3 days per week. Workers also unload ammonia from these containers following transportation. Process supervisors oversee the connection of pipes or hoses. Process supervision and pipe-hook up can be carried for 240 – 420 minutes per day, up to 100 times /year.

Workers involved in transferring ammonia into smaller containers, may typically spend 40-50 minutes filling drums or bottles, 10 times per shift. Workers controlling automatic, continuous or batch processes are segregated in separate control rooms. Processes may be carried out for 24 hours/day, up to 330 -360 days/year and require operators to cover 24 hours of continuous operation in shifts. Workers typically spend 80 % of a shift in a control room and 20 % of the time conducting field-based operations. Equipment is routinely inspected during tours lasting typically 2 hours/ shift, up to 50 days per year. Samples are taken for analysis and quality control (e.g. gas samples: 10 minutes / sample, 5 samples per shift; liquid ammonia samples: 15 minutes/sample, 1 per shift; ammonia product: 10 minutes/sample, 1 sample per week). Other tasks, such as maintenance work are carried out intermittently.

Although workers generally work standard shifts of 8 hours/day, longer shifts up to 12 hours/day may also be carried out.

1.2.1.3 Risk management measures

The formulation of aqueous ammonia solutions and the distribution of ammonia in aqueous and anhydrous forms involve special equipment and high integrity contained systems with little or no potential for worker exposure. Workers involved in controlling automated processes are segregated in separate control rooms with no direct contact with equipment. The potential for industrial workers to be exposed to ammonia when controlling processes is therefore negligible since they are located in a separate control room. Processes related to distribution or transportation activities are generally carried out outdoors, employing continuous, closed processes.

Workers may potentially be exposed to ammonia when operating equipment (e.g. valves, pumps or tanks etc). All operations are performed in a closed system. Pipelines and vessels are sealed and insulated and sampling is carried out with a closed sample loop. Extract ventilation is provided at openings and points were emissions may occur. Ammonia is stored in closed containers and tanks and transferred under containment. All technological devices have a proper quality certification, and are regularly controlled and maintained to avoid the uncontrolled discharge of ammonia.

Good occupational hygiene and exposure control measures are implemented to minimise the potential for worker exposure. Workers involved in formulation and distribution tasks are well-trained in these procedures and the use of appropriate protective equipment.

Where good natural ventilation is found to be inadequate, mechanical (general) ventilation or local exhaust ventilation (LEV) is provided. Road tankers are equipped with ventilation systems (e.g. an enclosing hood). Personal protective clothing (e.g. face/eye/ear protection, helmet, gloves boots and protective overall) is worn when any potential contact may arise. Workers unloading ammonia from storage or transportation vehicles wear tight fitting unvented goggles and a face shield to protect against splashes. Level A clothing (full encapsulating suit with self contained breathing apparatus) is used when handling large liquid spills or vapour clouds. Impervious clothing and rubber gloves are used for small liquid spills and normal loading and unloading operations. Safety shower/eye wash facilities are provided at sites which handle or store ammonia. Filtering respiratory masks are worn in case on the accidental release of ammonia.

1.2.2 Exposure estimation

1.2.2.1 Workers exposure

The assessment of worker exposure to aqueous ammonia during formulation or to anhydrous and aqueous forms of ammonia during distribution (ES 2) was carried out for processes relevant to this scenario as identified by PROC codes reflecting: use and storage of ammonia in closed systems with no likelihood of exposure (PROC 1), use in closed, continuous processes with occasional controlled exposure (PROC 2), formulation using closed batch processes (PROC 3), use in batch or other processes (PROC 4), mixing or blending in a batch process (PROC 5), maintenance and clean-down (PROC 8a), transfer (PROC 8b), transfer of ammonia into containers (PROC 9) and analysis of samples (PROC 15). A screening-level (Tier 1) assessment of worker exposure was carried out using the ECETOC Targeted Risk Assessment (TRA) model. The ECETOC TRA was used to predict dermal exposures (expressed as a daily systemic dose in mg/kg bw) and inhalation exposure concentrations (expressed as an airborne concentration in mg/m^3) associated with each process defined by PROC codes.

Exposure to workers was assessed taking into account different operational conditions that may be associated with the formulation of aqueous ammonia solutions and the distribution of anhydrous and aqueous ammonia products and the impact of different exposure control measures. Exposures were determined for task durations of 1- 4 hours or >4 hours and assuming that process are carried out either outdoors, indoors without use of local exhaust ventilation (LEV) or indoors with the use of LEV. To reflect the use of personal protective equipment (PPE), dermal exposures were determined assuming either no gloves or gloves affording 90% protection of the hands are worn. To reflect the use of respiratory protective equipment (RPE), inhalation exposure concentrations were determined assuming either no RPE or RPE affording 95% protection is worn.

The ECETOC TRA model uses a simple algorithm to determine dermal exposures that does not take the physical-chemical properties of a substance into account. The same dermal exposures where therefore predicted for anhydrous and aqueous forms of ammonia. Parameters used in the ECETOC TRA model to assess inhalation exposures were: molecular weight (35 $g.mol^{-1}$ and 17 $g.mol^{-1}$ for aqueous and anhydrous forms respectively and vapour pressure (the vapour pressure of anhydrous forms of ammonia is 8.6×10^5 Pa at 20^oC, whereas the vapour pressure of aqueous ammonia solution between 5 and 25% w/w ranges from 5×10^3 Pa to 4×10^4 Pa at 20^oC. Systemic dermal exposures have been determined for a worker with bodyweight 70 kg. ECETOC uses an algorithm.

1.2.2.1.1 Acute/Short term and long-term exposure

Potential systemic dermal exposures and inhalation exposure concentrations predicted by the ECETOC TRA model for the formulation of aqueous ammonia and the distribution of ammonia in anhydrous and aqueous forms are shown in Tables 23 and 24 respectively. ECETOC predicts a daily systemic dose following dermal exposure and a typical daily inhalation exposure concentration and does not specifically predict acute (short-term) and chronic (long-term) exposures. In the risk characterisation, dermal and inhalation exposures predicted by ECETOC are compared with acute and chronic DNEL values for local and systemic effects to determine the potential risk to human health associated with ES 2.

Table 23: Dermal exposures to anhydrous or aqueous (in preparations of 5-25 % w/w) ammonia predicted using the ECETOC TRA model for industrial workers involved in formulation or distribution (ES 2)

Description of activity	PROC	Exposure assumptions		Estimated Exposure Concentration mg/kg bw/d	
		Duration	Use of ventilation	No gloves worn	Gloves worn (90% reduction)
Used in a closed process, no likelihood of exposure: Storage (closed bulk or container)	PROC 1	1-4 hrs or >4 hrs	Outdoors /Indoors without LEV	0.34	0.03
Use in a closed, continuous process with occasional controlled exposure (e.g. sampling)	PROC 2	1-4 hrs or >4 hrs	Outdoors /Indoors without LEV	1.37	0.14
		1-4 hrs or >4 hrs	Indoors with LEV	0.14	0.01
Use in closed batch process (synthesis or formulation)	PROC 3	1-4 hrs or >4 hrs	Outdoors / Indoors without LEV	0.34	0.03
		1-4 hrs or >4 hrs	Indoors with LEV	0.03	<0.01
Use in batch process (synthesis) where opportunity for exposure arises	PROC 4	1-4 hrs or >4 hrs	Outdoors / Indoors without LEV	6.86	0.69
		1-4 hrs or >4 hrs	Indoors with LEV	0.69	0.07
Mixing or blending in batch process	PROC 5	1-4 hrs or >4 hrs	Outdoors / Indoors without LEV	13.71	1.37
		1-4 hrs or >4 hrs	Indoors with LEV	0.07	0.01
Maintenance, clean down	PROC 8a	1-4 hrs or >4 hrs	Outdoors / Indoors without LEV	13.71	1.37
		1-4 hrs or >4 hrs	Indoors with LEV	0.14	0.01
Transfer (charging/discharging) from/to vessels or large containers at dedicated facilities	PROC 8b	1-4 hrs or >4 hrs	Outdoors / Indoors without LEV	6.86	0.69
		1-4 hrs or >4 hrs	Indoors with LEV	0.69	0.07
Transfer into small containers	PROC 9	1-4 hrs or >4 hrs	Outdoors / Indoors without LEV	6.86	0.69
		1-4 hrs or >4 hrs	Indoors with LEV	0.69	0.07
Quality control in a laboratory	PROC 15	1-4 hrs or >4 hrs	Outdoors / Indoors without LEV	0.34	0.03
		1-4 hrs or >4 hrs	Indoors with LEV	0.03	<0.01

Table 24: Inhalation exposure concentrations for anhydrous ammonia predicted using the ECETOC TRA model for industrial workers involved in formulation or distribution (ES 2)

				Anhydrous ammonia		Aqueous ammonia (5-25% w/w)	
Description of activity	**PROC**	**Exposure assumptions**		**Estimated Exposure Concentration mg/m3**			
		Duration	**Use of ventilation**	**No RPE**	**RPE (95% reduction)**	**No RPE**	**RPE (95% reduction)**
Used in a closed process, no likelihood of exposure: Storage (closed bulk or container)	PROC 1	1-4 hrs or >4 hrs	Outdoors	0.00	NA	0.01	NA
		1-4 hrs or >4 hrs	Indoors without LEV	0.01	NA	0.01	NA
Use in a closed, continuous process with occasional controlled exposure (e.g. sampling)	PROC 2	>4hrs	Outdoors	24.79	1.24	30.63	1.53
		>4hrs	Indoors without LEV	35.42	1.77	43.75	2.19
		>4hrs	Indoors with LEV	3.53	0.18	4.38	0.22
		1-4 hrs	Outdoors	14.88	0.74	18.38	0.92
		1-4 hrs	Indoors without LEV	22.25	1.06	26.25	1.31
		1-4 hrs	Indoors with LEV	2.13	0.11	2.63	0.13
Use in closed batch process (synthesis or formulation)	PROC 3	>4hrs	Outdoors	49.58	2.48	61.25	3.06
		>4hrs	Indoors without LEV	70.83	3.54	87.5	4.38
		>4hrs	Indoors with LEV	7.08	0.35	8.75	0.44
		1-4 hrs	Outdoors	29.75	1.49	36.75	1.84
		1-4 hrs	Indoors without LEV	42.5	2.13	52.50	2.63
		1-4 hrs	Indoors with LEV	4.25	0.21	5.25	0.26
Use in batch process (synthesis) where opportunity for exposure arises	PROC 4	>4hrs	Outdoors	49.58	2.48	61.25	3.06
		>4hrs	Indoors without LEV	70.83	3.54	87.5	4.38
		>4hrs	Indoors with LEV	7.08	0.35	8.75	0.44
		1-4 hrs	Outdoors	29.75	1.49	36.75	1.84
		1-4 hrs	Indoors without LEV	42.5	2.13	52.5	2.63
		1-4 hrs	Indoors with LEV	4.25	0.21	5.25	0.26

Mixing or blending in batch process	PROC 5	>4hrs	Outdoors	123.96	6.20	153.13	7.66
		>4hrs	Indoors without LEV	177.08	8.85	218.75	10.94
		>4hrs	Indoors with LEV	17.71	0.89	21.88	1.09
		1-4 hrs	Outdoors	74.38	3.72	91.88	4.59
		1-4 hrs	Indoors without LEV	106.25	5.31	131.25	6.56
		1-4 hrs	Indoors with LEV	10.63	0.53	13.13	0.66
Maintenance, clean down	PROC 8a	>4hrs	Outdoors	123.96	6.20	153.13	7.66
		>4hrs	Indoors without LEV	177.08	8.85	218.75	10.94
		>4hrs	Indoors with LEV	17.71	0.89	21.88	1.09
		1-4 hrs	Outdoors	74.38	3.72	91.88	4.59
		1-4 hrs	Indoors without LEV	106.25	5.31	131.25	6.56
		1-4 hrs	Indoors with LEV	10.63	0.53	13.13	0.66
Transfer of ammonia (charging/discharging) from/to vessels or large containers at dedicated facilities	PROC 8b	>4hrs	Outdoors	74.38	3.72	91.88	4.59
		>4hrs	Indoors without LEV	106.25	5.31	131.25	6.56
		>4hrs	Indoors with LEV	3.19	0.16	3.94	0.20
		1-4 hrs	Outdoors	44.63	2.23	55.13	2.76
		1-4 hrs	Indoors without LEV	63.75	3.19	78.75	3.94
		1-4 hrs	Indoors with LEV	1.91	0.1	2.36	0.12
Transfer into small containers	PROC 9	>4hrs	Outdoors	99.17	4.96	122.50	6.13
		>4hrs	Indoors without LEV	141.67	7.08	175.00	8.75
		>4hrs	Indoors with LEV	14.17	0.71	17.50	0.88
		1-4 hrs	Outdoors	59.50	2.98	73.50	3.68
		1-4 hrs	Indoors without LEV	85.00	4.25	105.00	5.25
		1-4 hrs	Indoors with LEV	8.5	0.43	10.50	0.53
Quality control in a laboratory	PROC 15	>4hrs	Indoors without LEV	35.42	1.77	43.75	2.19
		>4hrs	Indoors with LEV	3.54	0.18	4.38	0.22
		1-4 hrs	Indoors without LEV	21.25	1.06	26.25	1.31
		1-4 hrs	Indoors with LEV	2.13	0.11	2.63	0.13

1.2.2.2 General public / consumer exposure

Formulation and distribution of ammonia is carried out at industrial sites from which members of the public are excluded. Members of the public will not therefore be exposed to ammonia during these processes. Consumer exposures to ammonia in the diluted (aqueous) form have been assessed in Section 1.6; ES 6.

1.2.2.3 Indirect exposure of humans via the environment (oral)

Ammonia is ubiquitous in the environment with <30% of emissions resulting from fertiliser uses and from non-agricultural sources (ref. 'Ammonia in the UK' - DEFRA).

In addition, there is no evidence that ammonia bioaccumulates as the log Kow value is 0.23. Since the trigger of BCF >100 (log Kow>3) is not met, the derivation of PNECs to protect against secondary poisoning is not required.

The risk of indirect exposure of humans via the environment is therefore not considered

1.2.2.4 Environmental exposure

First tier conservative environmental exposure estimations were carried out using EUSES 2.1 and with the specified defaults.

Second tier worst case environmental exposure estimations were carried out using EUSES 2.1 to take into account more realistic factors that affect the environmental concentrations.

1.2.2.4.1 Environmental releases

The environmental releases are determined primarily by tonnage and the ERC in the first tier with conservative estimations and defaults being implemented in EUSES. For the second and third tier assessments in EUSES, more realistic inputs were chosen to best suit the description of the production and uses of anhydrous ammonia. Emission defaults are those specified by the ECHA "Guidance on information requirements and chemical safety assessment: Chapter R.16: Environmental Exposure Estimation". Regional data and emission fractions were calculated using EUSES. Full EUSES inputs are shown below.

Table 25: EUSES inputs for environmental assessment

Input parameter:	Value:	Unit:	ERC default (if applicable)
Molecular Weight	35	g/mol	Value for aqueous ammonia used as it is this form which will predominate in the environment.
Vapour Pressure (at 20 °C)	287	hPa	Value for aqueous ammonia used as it is this form which will predominate in the environment.
Water Solubility	4.82 x 105	mg/L	
Octanol/water partition coefficient	0.23	logKow	
Koc	13.8		Modelled output used based on default 'non-hydrophobics' QSAR class within EUSES.
Biodegradability	Readily biodegradable		
Life Cycle Step	Industrial use		
Environmental Release Class	ERC 1		
Fraction of Tonnage for Region (1st Tier)			1
STP			Yes
Emission events per year	330	Days	Based on worst case emission events supplied by consortium members. Although, one consortium member reported emission days of 50, this was for a proportionately low tonnage and was not considered representative.
Default Release to Air for ERC 2	2.5	%	2.5
Default Release to Water for ERC 6B	2	%	2
Dilution factor applied for PEC derivation	10		10 (20,000 m^3/d)
Tonnage assessed	Total: 3,829,950 Regional: 1,000,000	tonnes/annum	Out of 21 combinations of uses and companies, 13 responses contained tonnage data. The total tonnage of 1717850 was normalized by a factor representing the number of companies in each use to estimate the total tonnage across the industry. Regional tonnage was taken to be the largest individual reported volume.

Table 26 Predicted Releases to the Environment Tier 1

ERC	Compartments	Predicted releases	Measured release	Explanation / source of measured data
2	Release to air	7.58×10^4 kg/day	-	Predicted values are those calculated by EUSES using the tonnage data and defaults for ERC2.
	Release to wastewater	6.06×10^4 kg/day	-	Predicted values are those calculated by EUSES using the tonnage data and defaults for ERC2.
	Soil (direct only) Agricultural soil	0	-	No direct loss to soil is expected for this ERC.

**The predicted releases were estimated using the EUSES 2.1 program.*

In reality removal of ammonia in sewage treatment plants is highly efficient being removed first by nitrification to nitrate followed by denitrification resulting in the release of nitrogen gas. Complete consumption within the STP can be assumed and this has been used in the tier 2 assessment within EUSES.

Table 27: Measured values for tier 2 assessment.

scriptionn of RMM	Details	Effect taken into account in EUSES	Comments
Efficient removal of ammonia in STP.	0 mg/L (Local) 0 kg/d (Regional)	Lowering of calculated concentration in STP effluent. Applied at both a local and a regional level. All regional emissions to STP.	

Table 28 Predicted Releases to the Environment Tier 2

ERC	Compartments	Predicted releases	Measured release	Explanation / source of measured data
2	Release to air	7.58×10^4 kg/day	-	Predicted values are those calculated by EUSES using the tonnage data and defaults for ERC 2
	Release to wastewater	6.06×10^4 kg/day	-	Predicted values are those calculated by EUSES using the tonnage data and defaults for ERC 2
	Soil (direct only) Agricultural soil	0	-	No direct loss to soil is expected for this ERC.

1.2.2.4.2 Exposure concentration in sewage treatment plants (STP)

Table 29: Tier 1 Concentrations in sewage

ERC for Compartment:	Estimated exposure concentrations		Measured exposure concentrations		Explanation / source of measured data
	Value	unit	value	unit	
Waste water before treatment	3.03×10^4	mg/L	NA	mg/L	
Sewage (STP effluent)	3.77×10^3	mg/L	NA	mg/L	
Local freshwater	377	mg/L	NA	mg/L	10-fold dilution by receiving waters

Table 30: Tier 2 Concentrations in sewage

ERC for Compartment:	Estimated exposure concentrations		Measured exposure concentrations		Explanation / source of measured data
	value	unit	value	unit	
Waste water before treatment	3.03×10^4	mg/L	NA	mg/L	
Sewage (STP effluent)	0	mg/L	NA	mg/L	Based on efficient removal by STP
Local freshwater	0	mg/L	NA	mg/L	10-fold dilution by receiving waters. Local concentration with atmospheric deposition not yet taken into account.

Table 31: General emission fractions from the municipal STP

Fraction description	Fraction amount	
	value	unit
Fraction of emission directed to air by STP	0.583	%
Fraction of emission directed to water by STP	12.4	%
Fraction of emission directed to sludge by STP	0.13	%
Fraction of emission degraded by STP	86.8	%

1.2.2.4.3 Exposure concentration in aquatic compartment

Table 32: Tier 1 Local concentrations in aquatic compartment

Compartments	Local concentration aquatic (local mg/L)	Justification
ERC2 Freshwater (in mg/L)	377	
ERC2 Marine water (in mg/L)	37	10-fold dilution by receiving waters
Intermittent releases to water (in mg/L)	NA	Intermittent release not relevant

Table 33: Tier 1 Predicted Environmental Concentrations (PEC) in aquatic compartment

Compartments	PEC aquatic (local mg/L)	Justification
ERC2Freshwater (in mg/L)	377	
ERC2 Marine water (in mg/L)	37	10-fold dilution by receiving waters
Intermittent releases to water (in mg/L)	NA	Intermittent release not relevant

Table 34: Tier 2 Local concentrations in aquatic compartment

Compartments	Local concentration aquatic (local mg/L)	Justification
Freshwater (in mg/L)	0	
Marine water (in mg/L)	00	10-fold dilution by receiving waters
Intermittent releases to water (in mg/L)	NA	Intermittent release not relevant

Table 35: Tier 2 Predicted Environmental Concentrations (PEC) in aquatic compartment

Compartments	PEC aquatic (local mg/L)	Justification
Freshwater (in mg/L)	1.3×10^{-3}	
Marine water (in mg/L)	3.14×10^{-4}	
Intermittent releases to water (in mg/L)	NA	Intermittent release not relevant

1.2.2.4.4 Exposure concentration in sediments

Table 36: Tier 1 Predicted Environmental Concentrations (PEC) in aquatic sediment compartment

Compartments	PEC aquatic (local)
ERC2 Freshwater sediment (in mg/kg)	408
ERC2 Marine sediment (in mg/kg)	40.8

Table 37: Tier 2 Predicted Environmental Concentrations (PEC) in aquatic sediment compartment

Compartments	PEC aquatic (local)
Freshwater sediment (in mg/kg)	1.41×10^{-3}
Marine sediment (in mg/kg)	3.40×10^{-4}

1.2.2.4.5 Exposure concentrations in soil and groundwater

Upon contact with soil, ammonia will be rapidly converted by a variety of bacteria, actinomycetes and fungi to ammonium (NH_4^+) by the process of ammonification or mineralization. Ammonium is then rapidly converted to nitrate. Nitrate is subsequently taken up and utilised by plants or returned to the atmosphere following denitrification; the metabolic reduction of nitrate into nitrogen or nitrous oxide (N2O) gas. The most likely fate of ammonium ions in soils is conversion to nitrates by nitrification. Therefore accumulation of concentrations of ammonia in soil and groundwater will not be expected.

1.2.2.4.6 Atmospheric compartment

Table 38: Tier 1 local concentrations in air

ERC		Estimated local exposure concentrations	Explanation / source of data
2	During emission (mg/m3)	21.1	Estimated using EUSES 2.1
	Annual average (mg/m3)	19.0	Estimated using EUSES 2.1
	Annual deposition (mg/m²/d)	27.5	Estimated using EUSES 2.1

Table 39: Tier 1 Predicted Exposure Concentration (PEC) in air

ERC		Local concentration	PEC air (local+regional)	Justification
2	Annual average PEC in air, total (mg/m3)	19.0	19.0	Estimated using EUSES 2.1.

Table 40: Tier 2 local concentrations in air

ERC		Estimated local exposure concentrations	Explanation / source of data
2	During emission (mg/m3)	21.1	Estimated using EUSES 2.1
	Annual average (mg/m3)	19.0	Estimated using EUSES 2.1
	Annual deposition (mg/m²/d)	27.5	Estimated using EUSES 2.1

Table 41: Tier 2 Predicted Exposure Concentration (PEC) in air

ERC		Local concentration	PEC air (local+regional)	Justification
2	Annual average PEC in air, total (mg/m3)	19.0	19.0	Estimated using EUSES 2.1.

1.2.2.4.7 Exposure concentration relevant for the food chain (Secondary poisoning)

In terms of secondary poisoning, there is no evidence that ammonia bioaccumulates as the log Kow value is 0.23. Since the trigger of BCF >100 (log Kow>3) is not met, the derivation of PNECs to protect against secondary poisoning is not required. Risk characterisation ratios cannot therefore be derived.

1.2.2.4.8 Regional exposure levels and environmental concentrations.

Anhydrous ammonia is produced and used at many sites throughout a region and this may lead to a degree of regional exposure. Regional exposure has been modelled for this exposure scenario using the regional module of EUSES 2.1.

Table 42: Tier 1 regional concentrations in the environment

	Predicted regional Exposure Concentrations		Measured regional exposure concentrations		Explanation / source of measured data
	PEC value	unit	Measured value	unit	
Freshwater	3.22×10^{-2}	mg/L	NA	mg/L	
Marine water	2.98×10^{-3}	mg/L	NA	mg/L	
Freshwater sediments	3.06×10^{-2}	mg/kg	NA	mg/kg	
Marine sediments	2.86×10^{-3}	mg/kg	NA	mg/kg	
Agricultural soil	7.14×10^{-4}	mg/kg	NA	mg/kg	
Grassland	9.29×10^{-4}	mg/kg	NA	mg/kg	
Air	1.42×10^{-3}	mg/m^3	NA	mg/m^3	

Table 43: Tier 2 regional concentrations in the environment

	Predicted regional Exposure Concentrations		Measured regional exposure concentrations		Explanation / source of measured data
	PEC value	unit	Measured value	unit	
Freshwater	1.30×10^{-3}	mg/L	NA	mg/L	
Marine water	3.14×10^{-4}	mg/L	NA	mg/L	
Freshwater sediments	1.24×10^{-3}	mg/kg	NA	mg/kg	
Marine sediments	3.02×10^{-4}	mg/kg	NA	mg/kg	
Agricultural soil	6.58×10^{-4}	mg/kg	NA	mg/kg	
Grassland	8.28×10^{-4}	mg/kg	NA	mg/kg	
Air	1.26×10^{-3}	mg/m^3	NA	mg/m^3	

1.3 Exposure Scenario 3: Industrial uses of anhydrous ammonia as an intermediate

1.3.1 Exposure scenario

Ammonia is used by the chemicals industry to manufacture a range other substances including: nitric acid, alkalis, dyes, pharmaceuticals, cosmetics, vitamins, synthetic textile fibres and plastics.

Ammonia is used as an intermediate in the synthesis of a number of chemicals. It is used in the manufacture of nitric acid (HNO_3) which is used in making explosives such as TNT (2,4,6-trinitrotoluene); nitro-glycerine (which is also used as a vasodilator) and PETN (pentaerythritol nitrate). Ammonia is also used in the synthesis of alkakis: sodium hydrogen carbonate (sodium bicarbonate; $NaHCO_3$), soda ash (sodium carbonate, Na_2CO_3), hydrogen cyanide (hydrocyanic acid; HCN) and hydrazine (N_2H_4) used in rocket propulsion systems.

Ammonia is used to manufacture explosives such as ammonium nitrate (NH_4NO_3). It is also used as an intermediate in the synthesis of dyes, and synthetic 'man-made' fibres such as nylon, rayon and acrylics. It is also used in the manufacture of plastics such as phenolics and polyurethanes.

Ammonia is used in the manufacture of drugs such as sulphonamide which inhibit the growth and multiplication of bacteria that require *p*-aminobenzoic acid (PABA) and for the biosynthesis of folic acids, antimalarials and vitamins (e.g. B vitamins: nicotinamide and thiamine).

Ammonia is also used in the production of ammonium and nitrate salts used in fertilisers.

1.3.1.1 Description of activities and processes covered in the exposure scenario

Processes using ammonia as an intermediate are carried out at large chemical manufacturing facilities. Due to the large size of these facilities, vessels and reactors for chemical synthesis and processing are housed outdoors. Some processes are carried out indoors. Processes are continuous or batch and are carried out in closed systems.

Most chemical manufacturing processes and units are operated automatically by a small number of operators located in separate control rooms. Operators may also carry out routine 'field' inspections around the facility to check that equipment is operating correctly. Other manual operations in the field may also be undertaken such as: preparation of equipment for mechanical or other work (e.g. maintenance), or taking samples or measurements. Workers unload ammonia stored in spheres onto tankers. Tanker unloading generally takes place in the open air and involves connecting or disconnecting pipes or hoses and opening or closing valves.

1.3.1.2 Operational conditions related to frequency and duration

Chemical processes using ammonia as an intermediate are closed, continuous or batch processes which can run for long periods without interruption indoors or outdoors, for up to 24 hours/day, 330-360 days per year. Operational control and some field operations such as inspection tours are therefore also carried out continuously (e.g. in shifts covering 24 hour periods daily, without interruption of the processes). Although operators generally work standard shifts of 8 hours/day and a normal working week, with production continuing at weekends, longer shifts up to 12 hours /day can also be carried out. Operators will typically work for 220 days/year. During a typical shift, operators may spend 80 % of their time in a control room and 20 % of their time in the field. Field operation tours can be up to 6 hours/shift, every day. Sampling (10 minutes/sample) for quality control is routinely carried out. Other activities such as maintenance work, are carried out intermittently. Workers also unload ammonia from transportation vehicles into containers. All processes are supervised.

1.3.1.3 Risk management measures

Chemical processes using ammonia as an intermediate involve special equipment and high integrity contained systems with little or no potential for worker exposure. These facilities are usually housed outdoors, with workers being segregated in separate control rooms with no direct contact with chemical processing units The potential for industrial workers to be exposed to ammonia during these processes is therefore negligible since they are located in separate control rooms.

Workers may potentially be exposed to ammonia when conducting field activities (e.g. when operating valves, pumps or tanks etc). All operations are performed in a closed system. Pipelines and vessels are sealed and insulated and sampling is carried out with a closed sample loop. Extract ventilation is provided at openings and points were emission may occur. Anhydrous ammonia is stored in closed containers and tanks. Ammonia is transferred under containment. A good standard of general or controlled ventilation is applied when maintenance activities are carried out. Personal protective clothing (e.g. face/eye protection, helmet, gloves, boots and protective overalls) is worn when any potential contact may arise.

All technological devices have a proper quality certification, and are regularly controlled and maintained to avoid the uncontrolled discharge of ammonia.

Good occupational hygiene and exposure control measures are implemented to minimise the potential for worker exposure. Workers involved in the manufacture, sampling and transfer of anhydrous ammonia to road tankers are well-trained in these procedures and use of appropriate protective equipment.

1.3.2 Exposure estimation

1.3.2.1 Workers exposure

The assessment of worker exposure to anhydrous and aqueous forms of ammonia used as an intermediate in chemical synthesis (ES 3) was carried out for processes relevant to this scenario as identified by PROC codes reflecting: use and storage of ammonia in closed systems with no likelihood of exposure (PROC 1), use in closed, continuous processes with occasional controlled exposure (PROC 2), formulation using closed batch processes (PROC 3), use in batch or other processes (PROC 4), mixing or blending in a batch process (PROC 5), maintenance and clean-down (PROC 8a), transfer (PROC 8b), transfer of ammonia into containers (PROC 9) and analysis of samples (PROC 15). A screening-level (Tier 1) assessment of worker exposure was carried out using the ECETOC Targeted Risk Assessment (TRA) model. The ECETOC TRA was used to predict dermal exposures (expressed as a daily systemic dose in mg/kg bw) and inhalation exposure concentrations (expressed as an airborne concentration in mg/m^3) associated with each process defined by PROC codes.

Exposure to workers was assessed taking into account different operational conditions that may be associated with the use of ammonia as an intermediate in chemical synthesis and the impact of different exposure control measures. Exposures were determined for task durations of 1- 4 hours or >4 hours and assuming that process are carried out either outdoors, indoors without use of local exhaust ventilation (LEV) or indoors with the use of LEV. To reflect the use of personal protective equipment (PPE), dermal exposures were determined assuming either no gloves or gloves affording 90% protection of the hands are worn. To reflect the use of respiratory protective equipment (RPE), inhalation concentrations were determined assuming either no RPE or RPE affording 95% protection is worn.

The ECETOC TRA model uses a simple algorithm to determine dermal exposures that does not take the physical-chemical properties of a substance into account. The same dermal exposure where therefore predicted for anhydrous and aqueous forms of ammonia. Parameters used in the ECETOC TRA model to assess inhalation exposures were: molecular weight (35 $g.mol^{-1}$ and 17 $g.mol^{-1}$ for aqueous and anhydrous forms respectively and vapour pressure (the vapour pressure of anhydrous forms of ammonia is 8.6×10^5 Pa at 20^oC, whereas the vapour pressure of aqueous ammonia solution between 5 and 25% w/w ranges from 5×10^3 Pa to 4×10^4 Pa at 20^oC. Systemic dermal exposures have been determined for a worker with bodyweight 70 kg.

1.3.2.1.1 Acute/Short term and long-term exposure

Potential systemic dermal exposures and inhalation exposure concentrations predicted by the ECETOC TRA model for processes associated with the use of ammonia in chemical synthesis are shown in Tables 44 and 45 respectively. ECETOC predicts a daily systemic dose following dermal exposure and a typical daily inhalation exposure concentration and does not specifically predict acute (short-term) and chronic (long-term) exposures. In the risk characterisation, dermal and inhalation exposures predicted by ECETOC are compared with acute and chronic DNEL values for local and systemic effects to determine the potential risk to human health associated with ES3.

Table 44: Dermal exposures to anhydrous or aqueous (in preparations of 5-25 % w/w) ammonia predicted using the ECETOC TRA model for industrial workers during chemical synthesis (ES 3)

Description of activity	PROC	Exposure assumptions		Estimated Exposure Concentration mg/kg bw/d	
		Duration	Use of ventilation	No gloves worn	Gloves worn (90% reduction)
Used in a closed process, no likelihood of exposure: Storage (closed bulk or container)	PROC 1	1-4 hrs or >4 hrs	Outdoors /Indoors without LEV	0.34	0.03
Use in a closed, continuous process with occasional controlled exposure (e.g. sampling)	PROC 2	1-4 hrs or >4 hrs	Outdoors /Indoors without LEV	1.37	0.14
		1-4 hrs or >4 hrs	Indoors with LEV	0.14	0.01
Use in closed batch process (synthesis or formulation)	PROC 3	1-4 hrs or >4 hrs	Outdoors / Indoors without LEV	0.34	0.03
		1-4 hrs or >4 hrs	Indoors with LEV	0.03	<0.01
Use in batch process (synthesis) where opportunity for exposure arises	PROC 4	1-4 hrs or >4 hrs	Outdoors / Indoors without LEV	6.86	0.69
		1-4 hrs or >4 hrs	Indoors with LEV	0.69	0.07
Mixing or blending in batch process	PROC 5	1-4 hrs or >4 hrs	Outdoors / Indoors without LEV	13.71	1.37
		1-4 hrs or >4 hrs	Indoors with LEV	0.07	0.01
Maintenance, clean down	PROC 8a	1-4 hrs or >4 hrs	Outdoors / Indoors without LEV	13.71	1.37
		1-4 hrs or >4 hrs	Indoors with LEV	0.14	0.01
Transfer (charging/discharging) from/to vessels or large containers at dedicated facilities	PROC 8b	1-4 hrs or >4 hrs	Outdoors / Indoors without LEV	6.86	0.69
		1-4 hrs or >4 hrs	Indoors with LEV	0.69	0.07
Transfer into small containers	PROC 9	1-4 hrs or >4 hrs	Outdoors / Indoors without LEV	6.86	0.69
		1-4 hrs or >4 hrs	Indoors with LEV	0.69	0.07
Quality control in a laboratory	PROC 15	1-4 hrs or >4 hrs	Outdoors / Indoors without LEV	0.34	0.03
		1-4 hrs or >4 hrs	Indoors with LEV	0.03	<0.01

Table 45: Inhalation exposure concentrations for anhydrous and aqueous (in preparations of 5-25 % w/w) ammonia predicted using the ECETOC TRA model for industrial workers during chemical synthesis (ES 3)

				Anhydrous ammonia		Aqueous ammonia (5-25% w/w)	
Description of activity	PROC	Exposure assumptions		Estimated Exposure Concentrations mg/m^3			
		Duration	Use of ventilation	No RPE	RPE (95% reduction)	No RPE	RPE (95% reduction)
Used in a closed process, no likelihood of exposure: Storage (closed bulk or container)	PROC 1	1-4 hrs or >4 hrs	Outdoors	0.00	NA	0.01	NA
		1-4 hrs or >4 hrs	Indoors without LEV	0.01	NA	0.01	NA
Use in a closed, continuous process with occasional controlled exposure (e.g. sampling)	PROC 2	>4hrs	Outdoors	24.79	1.24	30.63	1.53
		>4hrs	Indoors without LEV	35.42	1.77	43.75	2.19
		>4hrs	Indoors with LEV	3.53	0.18	4.38	0.22
		1-4 hrs	Outdoors	14.88	0.74	18.38	0.92
		1-4 hrs	Indoors without LEV	22.25	1.06	26.25	1.31
		1-4 hrs	Indoors with LEV	2.13	0.11	2.63	0.13
Use in closed batch process (synthesis or formulation)	PROC 3	>4hrs	Outdoors	49.58	2.48	61.25	3.06
		>4hrs	Indoors without LEV	70.83	3.54	87.5	4.38
		>4hrs	Indoors with LEV	7.08	0.35	8.75	0.44
		1-4 hrs	Outdoors	29.75	1.49	36.75	1.84
		1-4 hrs	Indoors without LEV	42.5	2.13	52.50	2.63
		1-4 hrs	Indoors with LEV	4.25	0.21	5.25	0.26
Use in batch process (synthesis) where opportunity for exposure arises	PROC 4	>4hrs	Outdoors	49.58	2.48	61.25	3.06
		>4hrs	Indoors without LEV	70.83	3.54	87.5	4.38
		>4hrs	Indoors with LEV	7.08	0.35	8.75	0.44
		1-4 hrs	Outdoors	29.75	1.49	36.75	1.84
		1-4 hrs	Indoors without LEV	42.5	2.13	52.5	2.63
		1-4 hrs	Indoors with LEV	4.25	0.21	5.25	0.26

Mixing or blending in batch process	PROC 5	>4hrs	Outdoors	123.96	6.20	153.13	7.66
		>4hrs	Indoors without LEV	177.08	8.85	218.75	10.94
		>4hrs	Indoors with LEV	17.71	0.89	21.88	1.09
		1-4 hrs	Outdoors	74.38	3.72	91.88	4.59
		1-4 hrs	Indoors without LEV	106.25	5.31	131.25	6.56
		1-4 hrs	Indoors with LEV	10.63	0.53	13.13	0.66
Maintenance, clean down	PROC 8a	>4hrs	Outdoors	123.96	6.20	153.13	7.66
		>4hrs	Indoors without LEV	177.08	8.85	218.75	10.94
		>4hrs	Indoors with LEV	17.71	0.89	21.88	1.09
		1-4 hrs	Outdoors	74.38	3.72	91.88	4.59
		1-4 hrs	Indoors without LEV	106.25	5.31	131.25	6.56
		1-4 hrs	Indoors with LEV	10.63	0.53	13.13	0.66
Transfer of ammonia (charging/discharging) from/to vessels or large containers at dedicated facilities	PROC 8b	>4hrs	Outdoors	74.38	3.72	91.88	4.59
		>4hrs	Indoors without LEV	106.25	5.31	131.25	6.56
		>4hrs	Indoors with LEV	3.19	0.16	3.94	0.20
		1-4 hrs	Outdoors	44.63	2.23	55.13	2.76
		1-4 hrs	Indoors without LEV	63.75	3.19	78.75	3.94
		1-4 hrs	Indoors with LEV	1.91	0.1	2.36	0.12
Transfer into small containers	PROC 9	>4hrs	Outdoors	99.17	4.96	122.50	6.13
		>4hrs	Indoors without LEV	141.67	7.08	175.00	8.75
		>4hrs	Indoors with LEV	14.17	0.71	17.50	0.88
		1-4 hrs	Outdoors	59.50	2.98	73.50	3.68
		1-4 hrs	Indoors without LEV	85.00	4.25	105.00	5.25
		1-4 hrs	Indoors with LEV	8.5	0.43	10.50	0.53
Quality control in a laboratory	PROC 15	>4hrs	Indoors without LEV	35.42	1.77	43.75	2.19
		>4hrs	Indoors with LEV	3.54	0.18	4.38	0.22
		1-4 hrs	Indoors without LEV	21.25	1.06	26.25	1.31
		1-4 hrs	Indoors with LEV	2.13	0.11	2.63	0.13

1.3.2.2 General public / consumer exposure

Industrial uses of anhydrous and aqueous ammonia are carried out at industrial sites from which members of the public are excluded. Members of the public will not be exposed to anhydrous or aqueous ammonia during industrial end-use. Consumer exposures to ammonia in the diluted (aqueous) from have been assessed in Section 1.6; ES 6.

1.3.2.3 Indirect exposure of humans via the environment (oral)

Ammonia is ubiquitous in the environment with <30% of emissions resulting from fertiliser uses and from non-agricultural sources (ref. 'Ammonia in the UK' - DEFRA).

In addition, there is no evidence that ammonia bioaccumulates as the log Kow value is 0.23. Since the trigger of BCF >100 (log Kow>3) is not met, the derivation of PNECs to protect against secondary poisoning is not required.

The risk of indirect exposure of humans via the environment is therefore not considered.

1.3.2.4 Environmental exposure

First tier conservative environmental exposure estimations were carried out using EUSES 2.1 and with the specified defaults.

Second tier worst case environmental exposure estimations were carried out using EUSES 2.1 to take into account more realistic factors that affect the environmental concentrations.

1.3.2.4.1 Environmental releases

The environmental releases are determined primarily by tonnage and the ERC in the first tier with conservative estimations and defaults being implemented in EUSES. For the second tier assessments in EUSES, more realistic inputs were chosen to best suit the description of the production and uses of anhydrous ammonia. Emission defaults are those specified by the ECHA "Guidance on information requirements and chemical safety assessment: Chapter R.16: Environmental Exposure Estimation". Regional data and emission fractions were calculated using EUSES. Full EUSES inputs are shown below.

Table 46: EUSES inputs for environmental assessment

Input parameter:	Value:	Unit:	ERC default (if applicable)
Molecular Weight	35	g/mol	Value for aqueous ammonia used as it is this form which will predominate in the environment.
Vapour Pressure (at 20 °C)	287	hPa	Value for aqueous ammonia used as it is this form which will predominate in the environment.
Water Solubility	4.82×10^5	mg/L	
Octanol/water partition coefficient	0.23	logKow	
Koc	13.8	L/kg	Modelled output used based on default 'non-hydrophobics' QSAR class within EUSES.
Biodegradability	Readily biodegradable		
Life Cycle Step	Industrial use		
Environmental Release Class	ERC 1		
Fraction of Tonnage for Region (1st Tier)			1
STP			Yes
Emission events per year	330	Days	Based on worst case emission events supplied by consortium members
Default Release to Air	ERC 6A: 5	%	ERC 6A: 5
Default Release to water	ERC 6A: 2	%	ERC 6A: 2
Dilution factor applied for PEC derivation	10		10 (20,000 m^3/d)

Tonnage assessed	Total: 3,829,950 Regional: 800,000	tonnes/annum	Of 12 consortium members, 6 responded with tonnage data for this scenario. The total of 1914975 tonnes was normalized by a factor representing the number of companies in each use to estimate the total tonnage across the industry. Regional tonnage was taken to be the largest individual reported volume.

Table 47 Predicted Releases to the Environment Tier 1

ERC	Compartments	Predicted releases	Measured release	Explanation / source of measured data
6A	Release to air	1.21×10^5 kg/day	-	Predicted values are those calculated by EUSES using the tonnage data and defaults for ERC6A.
	Release to wastewater	4.85×10^4 kg/day	-	Predicted values are those calculated by EUSES using the tonnage data and defaults for ERC6A.
	Soil (direct only) Agricultural soil	NA	-	No directly loss to soil is expected for this ERC.

**The predicted releases were estimated using the EUSES 2.1 program.*

In reality removal of ammonia in sewage treatment plants is highly efficient being removed first by nitrification to nitrate followed by denitrification resulting in the release of nitrogen gas. Complete consumption within the STP can be assumed and this has been used in the tier 2 assessment within EUSES.

Table 48: RMMs and measured values for tier 2 assessment.

Description of RMM	Details	Effect taken into account in EUSES	Comments
Efficient removal of ammonia in STP.	0 mg/L (Local) 0 kg/d (Regional)	Lowering of calculated concentration in STP effluent. Applied at both a local and a regional level. All regional emissions to STP.	

Table 49 Predicted Releases to the Environment Tier 2

ERC	Compartments	Predicted releases	Measured release	Explanation / source of measured data
6A	Release to air	1.21×10^5 kg/day	-	Predicted values are those calculated by EUSES using the tonnage data and defaults for ERC6A.
	Release to wastewater	4.85×10^4 kg/day	-	Predicted values are those calculated by EUSES using the tonnage data and defaults for ERC6A.
	Soil (direct only) Agricultural soil	NA	-	No direct loss to soil is expected for this ERC

1.3.2.4.2 Exposure concentration in sewage treatment plants (STP)

Table 50: Tier 1 Concentrations in sewage

ERC for Compartment:	Estimated exposure concentrations		Measured exposure concentrations		Explanation / source of measured data
	Value	unit	value	unit	
Waste water before treatment ERC 6A	2.42×10^{-4}	mg/L	NA	mg/L	
ERC 6A Sewage (STP effluent)	3.02×10^{3}	mg/L	NA	mg/L	
ERC 6A Local freshwater	302	mg/L	NA	mg/L	10-fold dilution by receiving waters

Table 51: Tier 2 Concentrations in sewage

ERC for Compartment:	Estimated exposure concentrations		Measured exposure concentrations		Explanation / source of measured data
	Value	unit	value	unit	
Waste water before treatment ERC 6A	2.42×10^{-4}	mg/L	NA	mg/L	
ERC 6A Sewage (STP effluent)	0	mg/L	NA	mg/L	Based on efficient removal by STP
ERC 6A Local freshwater	0	mg/L	NA	mg/L	10-fold dilution by receiving waters

Table 52: General emission fractions from the municipal STP

Fraction description	Fraction amount	
	value	unit
Fraction of emission directed to air by STP	0.583	%
Fraction of emission directed to water by STP	12.4	%
Fraction of emission directed to sludge by STP	0.13	%
Fraction of emission degraded by STP	86.8	%

1.3.2.4.3 Exposure concentration in aquatic pelagic compartment

Table 53: Tier 1 Local concentrations in aquatic compartment

Compartments	Local concentration aquatic (local mg/L)	Justification
ERC6A Freshwater (in mg/L)	302	
ERC6A Marine water (in mg/L)	30.2	10-fold dilution by receiving waters

Table 54: Tier 1 Predicted Environmental Concentrations (PEC) in aquatic compartment

Compartments	PEC aquatic (local mg/L)	Justification
ERC6A Freshwater (in mg/L)	302	
ERC 6A Marine water (in mg/L)	30.2	10-fold dilution by receiving waters

Table 55: Tier 2 Local concentrations in aquatic compartment

Compartments	Local concentration aquatic (local mg/L)	Justification
ERC6A Freshwater (in mg/L)	0	
ERC6A Marine water (in mg/L)	0	10-fold dilution by receiving waters

Table 56: Tier 2 Predicted Environmental Concentrations (PEC) in aquatic compartment

Compartments	PEC aquatic (local mg/L)	Justification
ERC6A Freshwater (in mg/L)	2.19×10^{-3}	
ERC6A Marine water (in mg/L)	5.37×10^{-4}	

1.3.2.4.4 Exposure concentration in sediments

Table 57: Tier 1 Predicted Environmental Concentrations (PEC) in aquatic sediment compartment

Compartments	PEC aquatic (local)
ERC6A Freshwater sediment (in mg/kg)	327
ERC6A Marine sediment (in mg/kg)	32.7

Table 58: Tier 2 Predicted Environmental Concentrations (PEC) in aquatic sediment compartment

Compartments	PEC aquatic (local)
ERC6A Freshwater sediment (in mg/kg)	2.37×10^{-3}
ERC6A Marine sediment (in mg/kg)	5.82×10^{-4}

1.3.2.4.5 Exposure concentrations in soil and groundwater

Upon contact with soil, ammonia will be rapidly converted by a variety of bacteria, actinomycetes and fungi to ammonium (NH_4^+) by the process of ammonification or mineralization. Ammonium is then rapidly converted to nitrate. Nitrate is subsequently taken up and utilised by plants or returned to the atmosphere following denitrification; the metabolic reduction of nitrate into nitrogen or nitrous oxide (N2O) gas. The most likely fate of ammonium ions in soils is conversion to nitrates by nitrification. Therefore accumulation of concentrations of ammonia in soil and groundwater will not be expected.

1.3.2.4.6 Atmospheric compartment

Table 59: Tier 1 local concentrations in air

ERC		Estimated local exposure concentrations	Explanation / source of data
6A	During emission (mg/m3)	33.7	Estimated using EUSES 2.1
	Annual average (mg/m3)	30.5	Estimated using EUSES 2.1
	Annual deposition (mg/m²/d)	43.9	Estimated using EUSES 2.1

Table 60: Tier 1 Predicted Exposure Concentration (PEC) in air

ERC		Local concentration	PEC air (local+regional)	Justification
6A	Annual average PEC in air, total (mg/m3)	30.5	30.5	Estimated using EUSES 2.1.

Table 61: Tier 2 local concentrations in air

ERC		Estimated local exposure concentrations	Explanation / source of data
6A	During emission (mg/m3)	33.7	Estimated using EUSES 2.1
	Annual average (mg/m3)	30.5	Estimated using EUSES 2.1
	Annual deposition (mg/m²/d)	43.8	Estimated using EUSES 2.1

Table 62: Tier 2 Predicted Exposure Concentration (PEC) in air

ERC		Local concentration	PEC air (local+regional)	Justification
6A	Annual average PEC in air, total (mg/m3)	30.5	30.5	Estimated using EUSES 2.1.

1.3.2.4.7 Exposure concentration relevant for the food chain (Secondary poisoning)

In terms of secondary poisoning, there is no evidence that ammonia bioaccumulates as the log Kow value is 0.23. Since the trigger of BCF >100 (log Kow>3) is not met, the derivation of PNECs to protect against secondary poisoning is not required. Risk characterisation ratios cannot therefore be derived.

1.3.2.4.8 Regional exposure levels and environmental concentrations.

Anhydrous ammonia is produced and used at many sites throughout a region and this may lead to a degree of regional exposure. Regional exposure has been modelled for this exposure scenario using the regional module of EUSES 2.1.

Table 63: Tier 1 regional concentrations in the environment

	Predicted regional Exposure Concentrations		Measured regional exposure concentrations		Explanation / source of measured data
	PEC value	unit	Measured value	unit	
ERC 6a Freshwater	2.68×10^{-2}	mg/L	NA	mg/L	
ERC 6a Marine water	2.67×10^{-3}	mg/L	NA	mg/L	
ERC 6a Freshwater sediments	2.56×10^{-2}	mg/kg	NA	mg/kg	
ERC 6a Marine sediments	2.56×10^{-3}	mg/kg	NA	mg/kg	
ERC 6a Agricultural soil	1.00×10^{-3}	mg/kg	NA	mg/kg	
ERC 6a Grassland	1.47×10^{-3}	mg/kg	NA	mg/kg	
ERC 6a Air	2.24×10^{-3}	mg/m^3	NA	mg/m^3	

Table 64: Tier 2 regional concentrations in the environment

	Predicted regional Exposure Concentrations		Measured regional exposure concentrations		Explanation / source of measured data
	PEC value	unit	Measured value	unit	
ERC 6a Freshwater	2.19×10^{-3}	mg/L	NA	mg/L	
ERC 6a Marine water	5.37×10^{-4}	mg/L	NA	mg/L	
ERC 6a Freshwater sediments	2.09×10^{-3}	mg/kg	NA	mg/kg	
ERC 6a Marine sediments	5.15×10^{-4}	mg/kg	NA	mg/kg	
ERC 6a Agricultural soil	9.88×10^{-4}	mg/kg	NA	mg/kg	
ERC 6a Grassland	1.39×10^{-3}	mg/kg	NA	mg/kg	
ERC 6a Air	2.12×10^{-3}	mg/m^3	NA	mg/m^3	

1.4 Exposure Scenario 4: Industrial end-use of anhydrous and aqueous ammonia (processing, non-processing aids, auxiliary agent)

1.4.1 Exposure scenario

Anhydrous liquid and aqueous solutions of ammonia are used by a range of industry sectors in a broad number of applications. These include industrial use as a reactive or non-reactive processing aid in continuous or batch processes, as an auxiliary agent or as substance in a closed system. Common industrial end-uses of ammonia are shown in table 65.

Table 65: Common industrial end-uses of ammonia

Industrial end-use	Type of use					Description of use
	Processing aid	Non-processing aid	Reactive processing aid	Auxiliary agent	Use in closed system	
Use as developing agent in photochemical processes	X					Ammonia is used as a developing agent in photochemical processes such as white printing, blue printing and in the diazo duplication press.
Use of refrigerant systems		X			X	Anhydrous liquid ammonia is used as a refrigerant in household, commercial and industrial systems due to its high heat of vaporisation and relative ease of liquefaction.
Insulation products		X				
Inks and toners	X	X				Ammonia vapours are used as a reagent in treating writing or ink marks
Coatings, thinners, paint removers	X	X				
Processing aid in chemicals industry			X			
Use as an extraction agent			X			Ammonia is used as an extraction agent in the mining industry to extract metals like copper, nickel and molybdenum from their ores.
Treatment of gas (NOx and SOx reduction)			X		X	Ammonia is used in stack emission control systems to neutralise sulphur oxides from combustion of sulphur-containing fuels, as a method of NOx control in both catalytic and non-catalytic applications and to enhance the efficiency of electrostatic precipitators for particulate control.
Processing aid in nutrition			X		X	The food and beverage industry use ammonia as a source of nitrogen required for yeast and micro-organism
Use as neutralising agent			X		X	Ammonia is used by the petrochemical industry in neutralizing the acid constituents of crude oil and in the protection of equipment from corrosion
Textile dyes			X			

Treatment of water	X		X			Aqueous ammonia is used in water and waste-water treatment areas to control pH, to regenerate weak anion exchange resins and as an oxygen scavenger in boiled water treatment. In water disinfection, aqueous ammonia is added to water containing free chlorine to produce a chloramines disinfectant.
Use as washing and cleaning products	X		X			Weak ammonia solutions are used extensively within industry, by professionals and consumers as commercial and household cleaners and detergents cleaning products. Commercial ammonia cleaning products contain up to 30% ammonia whereas household products contain 5-10% ammonia
Treatment of textiles		X	X			Liquid ammonia is used to increase the quality of textiles
Treatment of pulp and paper		X	X			Ammonia is used in the pulp and paper industry to pulp wood and as a casein dispersant to coat paper.
Treatment of leather		X	X			The leather industry utilises ammonia as a curing agent, as a slime and mould preservative in tanning liquors and as a protective agent for leather and furs in storage
Treatment of wood	X		X			Anhydrous ammonia fumes are used to darken wood in a process called "ammonia fuming"
Treatment of metal surfaces	X		X			Ammonia is used in metal treatment processes such as nitriding, carbonitriding, bright annealing, furnace brazing, sintering, sodium hydride descaling, atomic hydrogen welding and other application where protective atmospheres are required.
Treatment of rubber/latex		X	X			Concentrated aqueous ammonia is used in the rubber industry as a preservative for natural and synthetic latex due to its antibacterial and alkaline properties and as a stabiliser to prevent pre-mature coagulation (e.g. "ammoniation" of natural rubber latex.
Manufacture of semiconductors/electronics				X		Ammonia is used in the electronics industry in the manufacturing of semiconductor chips.
Adhesives, sealants	X			X		
Polymer preparations	X			X		
Aircare products					X	
Preservatives		X				Ammonia is uses as a preservative for the storage of high moisture corn

1.4.1.1 Description of activities and processes covered in the exposure scenario

Operational conditions pertaining to the broad range of industrial end-use scenarios involving anhydrous and aqueous forms of ammonia vary considerably across applications and industrial sector of use. A full characterisation of the frequency and duration of tasks is beyond the scope of this report. For the purpose of worker exposure estimation, activities and processes associated with the industrial end-use of ammonia have been represented generically, based on the process categories (e.g. PROC codes) defined by REACH guidance. Processes and activities relevant to ES 4 are described as: use and storage of ammonia in closed systems with no likelihood of exposure (PROC 1), use in close, continuous process with occasional controlled exposure (PROC 2), formulation using closed batch processes (PROC 3), use in batch or other processes (PROC 4), mixing or blending in a batch process (PROC 5), industrial spraying (PROC 7), maintenance and clean down (PROC 8a), transfer (PROC 8b), transfer of ammonia into containers (PROC 9), brush and roller applications (PROC 10), treatment of articles by dipping and pouring (PROC 13), and analysis of samples (PROC 15) and hand-mixing (PROC 19).

1.4.1.2 Operational conditions related to frequency and duration of use

Operational conditions pertaining to the broad range of industrial end-use scenarios involving anhydrous and aqueous forms of ammonia vary considerably across applications and industrial sector of use. A full characterisation of the frequency and duration of tasks is beyond the scope of this report. For the purposes of worker exposure estimation, operational conditions have been represented generically based on the assumptions that tasks may be either 1-4 hours or >4 hours in duration and processes can be carried out either outdoors, indoors without LEV or indoors with LEV.

1.4.1.3 Risk management measures

Industrial end-uses of anhydrous and aqueous forms of ammonia involve special equipment and high integrity contained systems with little or no potential for worker exposure. Facilities may be housed outdoors, with workers being segregated in separate control rooms with no direct contact with chemical processing units The potential for industrial workers to be exposed to ammonia during these processes is therefore negligible since they are located in a separate control room.

Workers may potentially be exposed to ammonia when conducting field activities (e.g. when operating valves, pumps or tanks etc). All operations are performed in a closed system. Pipelines and vessels are sealed and insulated and sampling is carried out with a closed sample loop. Extract ventilation is provided at openings and points were emission may occur. Anhydrous ammonia is stored in closed containers and tanks. Ammonia is transferred under containment. A good standard of general or controlled ventilation is applied when maintenance activities are carried out. Personal protective clothing (e.g. face/eye protection, helmet, gloves, boots and protective overalls) is worn when any potential contact may arise.

All technological devices have a proper quality certification, and are regularly controlled and maintained to avoid the uncontrolled discharge of ammonia.

Good occupational hygiene and exposure control measures are implemented to minimise the potential for worker exposure. Workers involved in the manufacture, sampling and transfer of anhydrous ammonia to road tankers are well-trained in these procedures and use of appropriate protective equipment.

1.4.2 Exposure estimation

The assessment of worker exposure to anhydrous and aqueous forms of ammonia in industrial end-use applications (ES 4) was carried out for processes relevant to this scenario as identified by PROC codes reflecting: use and storage of ammonia in closed systems with no likelihood of exposure (PROC 1), use in closed, continuous processes with occasional controlled exposure (PROC 2), formulation using closed batch processes (PROC 3), use in batch or other processes (PROC 4), mixing or blending in a batch process (PROC 5), industrial spraying (PROC 7), maintenance and clean down (PROC 8a), transfer (PROC 8b), transfer of ammonia into containers (PROC 9), brush and roller applications (PROC 10), treatment of articles by dipping and pouring (PROC 13), and analysis of samples (PROC 15) and hand-mixing (PROC 19).

A screening-level (Tier 1) assessment of worker exposure was carried out using the ECETOC Targeted Risk Assessment (TRA) model. The ECETOC TRA was used to predict dermal exposures (expressed as a daily systemic dose in mg/kg bw) and inhalation exposure concentrations (expressed as an airborne concentration in mg/m3) associated with each process defined by PROC codes.

Exposure to workers was assessed taking into account different operational conditions that may be associated with the industrial end-use of ammonia and the impact of different exposure control measures. Exposures were determined for task durations of 1- 4 hours or >4 hours and assuming that process are carried out either outdoors, indoors without use of local exhaust ventilation (LEV) or indoors with the use of LEV. To reflect the use of personal protective equipment (PPE), dermal exposures were determined assuming either no gloves or gloves affording 90% protection of the hands are worn. To reflect the use of respiratory protective equipment (RPE), inhalation exposure concentrations were determined assuming either no RPE or RPE affording 95% protection is worn.

The ECETOC TRA model uses a simple algorithm to determine dermal exposures that does not take the physical-chemical properties of a substance into account. The same dermal exposure where therefore predicted for anhydrous and aqueous forms of ammonia. Parameters used in the ECETOC TRA model to assess inhalation exposures were: molecular weight (35 $g.mol^{-1}$ and 17 $g.mol^{-1}$ for aqueous and anhydrous forms respectively) and vapour pressure (the vapour pressure of anhydrous forms of ammonia is 8.6×10^5 Pa at 20°C, whereas the vapour pressure of aqueous ammonia solution between 5 and 25% w/w ranges from 5×10^3 Pa to 4×10^4 Pa at 20°C. Systemic dermal exposures have been determined for a worker with bodyweight 70 kg.

1.4.2.1.1 Acute/Short term and long-term exposure

Potential systemic dermal exposures and inhalation exposure concentrations predicted by the ECETOC TRA model for the industrial end-use of ammonia are shown in Tables 66 and 67 respectively. ECETOC predicts a daily systemic dose following dermal exposure and a typical daily inhalation exposure concentration and does not specifically predict acute (short-term) and chronic (long-term) exposures. In the risk characterisation, dermal and inhalation exposures predicted by ECETOC are compared with acute and chronic DNEL values for local and systemic effects to determine the potential risk to human health associated with ES 4.

Table 66: Dermal exposures to anhydrous or aqueous (in preparations of 5-25 % w/w) ammonia predicted using the ECETOC TRA model for industrial workers during industrial-end use processes (ES 4)

Description of activity	PROC	Exposure assumptions		Estimated Exposure Concentration mg/kg bw/d	
		Duration	Use of ventilation	No gloves worn	Gloves worn (90% reduction)
Used in a closed process, no likelihood of exposure: Storage (closed bulk or container)	PROC 1	1-4 hrs or >4 hrs	Outdoors /Indoors without LEV	0.34	0.03
Use in a closed, continuous process with occasional controlled exposure (e.g. sampling)	PROC 2	1-4 hrs or >4 hrs	Outdoors /Indoors without LEV	1.37	0.14
		1-4 hrs or >4 hrs	Indoors with LEV	0.14	0.01
Use in closed batch process (synthesis or formulation)	PROC 3	1-4 hrs or >4 hrs	Outdoors / Indoors without LEV	0.34	0.03
		1-4 hrs or >4 hrs	Indoors with LEV	0.03	<0.01
Use in batch process (synthesis) where opportunity for exposure arises	PROC 4	1-4 hrs or >4 hrs	Outdoors / Indoors without LEV	6.86	0.69
		1-4 hrs or >4 hrs	Indoors with LEV	0.69	0.07
Mixing or blending in batch process	PROC 5	1-4 hrs or >4 hrs	Outdoors / Indoors without LEV	13.71	1.37
		1-4 hrs or >4 hrs	Indoors with LEV	0.07	0.01
Industrial spraying	PROC 7	1-4 hrs or >4 hrs	Outdoors / Indoors without LEV	42.86	4.29
		1-4 hrs or >4 hrs	Indoors with LEV	2.14	0.21
Maintenance, clean down	PROC 8a	1-4 hrs or >4 hrs	Outdoors / Indoors without LEV	13.71	1.37
		1-4 hrs or >4 hrs	Indoors with LEV	0.14	0.01

Transfer (charging/discharging) from/to vessels or large containers at dedicated facilities	PROC 8b	1-4 hrs or >4 hrs	Outdoors / Indoors without LEV	6.86	0.69
		1-4 hrs or >4 hrs	Indoors with LEV	0.69	0.07
Transfer into small containers	PROC 9	1-4 hrs or >4 hrs	Outdoors / Indoors without LEV	6.86	0.69
		1-4 hrs or >4 hrs	Indoors with LEV	0.69	0.07
Roller application or brushing	PROC 10	1-4 hrs or >4 hrs	Outdoors / Indoors without LEV	27.43	2.74
		1-4 hrs or >4 hrs	Indoors with LEV	1.37	0.14
Treatment of articles by dipping and pouring	PROC 13	1-4 hrs or >4 hrs	Outdoors / Indoors without LEV	13.71	1.37
		1-4 hrs or >4 hrs	Indoors with LEV	0.69	0.07
Quality control in a laboratory	PROC 15	1-4 hrs or >4 hrs	Outdoors / Indoors without LEV	0.34	0.03
		1-4 hrs or >4 hrs	Indoors with LEV	0.03	<0.01
And-mixing with intimate contact and PPE only	PROC 19	1-4 hrs or >4 hrs	Outdoors / Indoors without LEV	141.73	14.13

Table 67: Inhalation exposure concentrations for anhydrous and aqueous (in preparations of 5-25 % w/w) ammonia predicted using the ECETOC TRA model for industrial workers during industrial end-use processes (ES 4)

Description of activity	PROC	Exposure assumptions		Anhydrous ammonia		Aqueous ammonia (5-25% w/w)	
				Estimated Exposure Concentration mg/m3		Estimated Exposure Concentration mg/m3	
		Duration	Use of ventilation	No RPE	RPE (95% reduction)	No RPE	RPE (95% reduction)
Used in a closed process, no likelihood of exposure	PROC 1	1-4 hrs or >4 hrs	Outdoors	0.00	NA	0.01	0.00
		1-4 hrs or >4 hrs	Indoors without LEV	0.01	NA	0.01	0.00
Use of ammonia in a closed, continuous process with occasional controlled exposure (e.g. sampling)	PROC 2	>4hrs	Outdoors	24.79	1.24	30.63	1.53
		>4hrs	Indoors without LEV	35.42	1.77	43.75	2.19
		>4hrs	Indoors with LEV	3.53	0.18	4.38	0.22
		1-4 hrs	Outdoors	14.88	0.74	18.38	0.92
		1-4 hrs	Indoors without LEV	22.25	1.06	26.25	1.31
		1-4 hrs	Indoors with LEV	2.13	0.11	2.63	0.13

Use of ammonia in closed batch process (synthesis or formulation)	PROC 3	>4hrs	Outdoors	49.58	2.48	61.25	3.06
		>4hrs	Indoors without LEV	70.83	3.54	87.5	4.38
		>4hrs	Indoors with LEV	7.08	0.35	8.75	0.44
		1-4 hrs	Outdoors	29.75	1.49	36.75	1.84
		1-4 hrs	Indoors without LEV	42.5	2.13	52.50	2.63
		1-4 hrs	Indoors with LEV	4.25	0.21	5.25	0.26
Use of ammonia in batch process (synthesis) where opportunity for exposure arises	PROC 4	>4hrs	Outdoors	49.58	2.48	61.25	3.06
		>4hrs	Indoors without LEV	70.83	3.54	87.5	4.38
		>4hrs	Indoors with LEV	7.08	0.35	8.75	0.44
		1-4 hrs	Outdoors	29.75	1.49	36.75	1.84
		1-4 hrs	Indoors without LEV	42.5	2.13	52.5	2.63
		1-4 hrs	Indoors with LEV	4.25	0.21	5.25	0.26
Mixing or blending in batch process	PROC 5	>4hrs	Outdoors	123.96	6.20	153.13	7.66
		>4hrs	Indoors without LEV	177.08	8.85	218.75	10.94
		>4hrs	Indoors with LEV	17.71	0.89	21.88	1.09
		1-4 hrs	Outdoors	74.38	3.72	91.88	4.59
		1-4 hrs	Indoors without LEV	106.25	5.31	131.25	6.56
		1-4 hrs	Indoors with LEV	10.63	0.53	13.13	0.66
Industrial spraying	PROC 7	>4hrs	Outdoors	NA	NA	306.25	15.31
		>4hrs	Indoors without LEV	NA	NA	437.5	21.88
		>4hrs	Indoors with LEV	NA	NA	21.88	1.09
		1-4 hrs	Outdoors	NA	NA	183.75	9.19
		1-4 hrs	Indoors without LEV	NA	NA	262.5	13.13
		1-4 hrs	Indoors with LEV	NA	NA	13.13	0.66

Transfer of ammonia (charging/discharging) from/to vessels or large containers at non-dedicated facilities	PROC 8a	>4hrs	Outdoors	123.96	6.20	153.13	7.66
		>4hrs	Indoors without LEV	177.08	8.85	218.75	10.94
		>4hrs	Indoors with LEV	17.71	0.89	21.88	1.09
		1-4 hrs	Outdoors	74.38	3.72	91.88	4.59
		1-4 hrs	Indoors without LEV	106.25	5.31	131.25	6.56
		1-4 hrs	Indoors with LEV	10.63	0.53	13.13	0.66
Transfer of ammonia (charging/discharging) from/to vessels or large containers at dedicated facilities	PROC 8b	>4hrs	Outdoors	74.38	3.72	91.88	4.59
		>4hrs	Indoors without LEV	106.25	5.31	131.25	6.56
		>4hrs	Indoors with LEV	3.19	0.16	3.94	0.20
		1-4 hrs	Outdoors	44.63	2.23	55.13	2.76
		1-4 hrs	Indoors without LEV	63.75	3.19	78.75	3.94
		1-4 hrs	Indoors with LEV	1.91	0.1	2.36	0.12
Transfer of ammonia into small containers	PROC 9	>4hrs	Outdoors	99.17	4.96	122.50	6.13
		>4hrs	Indoors without LEV	141.67	7.08	175.00	8.75
		>4hrs	Indoors with LEV	14.17	0.71	17.50	0.88
		1-4 hrs	Outdoors	59.50	2.98	73.50	3.68
		1-4 hrs	Indoors without LEV	85.00	4.25	105.00	5.25
		1-4 hrs	Indoors with LEV	8.5	0.43	10.50	0.53
Roller application or brushing	PROC 10	>4hrs	Outdoors	NA	NA	153.13	7.66
		>4hrs	Indoors without LEV	NA	NA	218.75	10.94
		>4hrs	Indoors with LEV	NA	NA	21.88	1.09
		1-4 hrs	Outdoors	NA	NA	91.88	4.59
		1-4 hrs	Indoors without LEV	NA	NA	131.25	6.56
		>4hrs	Outdoors	NA	NA	13.13	0.66
Treatment of articles by dipping and pouring	PROC 13	>4hrs	Outdoors	123.96	6.20	153.13	7.66
		>4hrs	Indoors without LEV	177.08	8.85	218.75	10.94
		>4hrs	Indoors with LEV	17.71	0.89	21.88	1.09
		1-4 hrs	Outdoors	74.38	3.72	91.88	4.59
		1-4 hrs	Indoors without LEV	106.25	5.31	131.25	6.56
		1-4 hrs	Indoors with LEV	10.63	0.53	13.13	0.66

Use as a laboratory agent	PROC 15	>4hrs	Indoors without LEV	35.42	1.77	43.75	2.19
		>4hrs	Indoors with LEV	3.54	0.18	4.38	0.22
		1-4 hrs	Indoors without LEV	21.25	1.06	26.25	1.31
		1-4 hrs	Indoors with LEV	2.13	0.11	2.63	0.13
Hand-mixing with intimate contact and PPE only	PROC 19	<4 hrs	Outdoors	NA	NA	153.13	7.66
		<4 hrs	Indoors without LEV	NA	NA	218.75	10.94
		1-4 hrs	Outdoors	NA	NA	91.88	4.59
		1-4 hrs	Indoors without LEV	NA	NA	131.25	6.56

1.4.2.2 General public / consumer exposure

Industrial uses of anhydrous and aqueous ammonia are carried out at industrial sites from which members of the public are excluded. Members of the public will not be exposed to anhydrous or aqueous ammonia during industrial end-use. Consumer exposures to ammonia in the diluted (aqueous) from have been assessed in Section 1.6; ES 6.

1.4.2.3 Indirect exposure of humans via the environment (oral)

Ammonia is ubiquitous in the environment with <30% of emissions resulting from fertiliser uses and from non-agricultural sources (ref. 'Ammonia in the UK' - DEFRA).

In addition, there is no evidence that ammonia bioaccumulates as the log Kow value is 0.23. Since the trigger of BCF >100 (log Kow>3) is not met, the derivation of PNECs to protect against secondary poisoning is not required.

The risk of indirect exposure of humans via the environment is therefore not considered.

1.4.2.4 Environmental exposure

First tier conservative environmental exposure estimations were carried out using EUSES 2.1 and with the specified defaults.

Second tier worst case environmental exposure estimations were carried out using EUSES 2.1 to take into account more realistic factors that affect the environmental concentrations.

1.4.2.4.1 Environmental releases

The environmental releases are determined primarily by tonnage and the ERC in the first tier with conservative estimations and defaults being implemented in EUSES. For the second tier assessments in EUSES, more realistic inputs were chosen to best suit the description of the production and uses of anhydrous ammonia. Emission defaults are those specified by the ECHA "Guidance on information requirements and chemical safety assessment: Chapter R.16: Environmental Exposure Estimation". Regional data and emission fractions were calculated using EUSES. Full EUSES inputs are shown below.

Table 68: EUSES inputs for ES4

Input parameter:	Value:	Unit:	ERC default (if applicable)
Molecular Weight	35	g/mol	Value for aqueous ammonia used as it is this form which will predominate in the environment.
Vapour Pressure (at 20 °C)	287	hPa	Value for aqueous ammonia used as it is this form which will predominate in the environment.
Water Solubility	4.82 x 10^5	mg/L	
Octanol/water partition coefficient	0.23	logKow	
Koc	13.8	L/kg	Modelled output used based on default 'non-hydrophobics' QSAR class within EUSES.
Biodegradability	Readily biodegradable		
Life Cycle Step	Industrial use		
Environmental Release Class	ERC 4, 5, 6B, 6D and 7		
Fraction of Tonnage for Region (1st Tier)	0.7		1 Fraction chosen to reflect largest user
STP	Yes		Yes
Emission events per year	330	Days	Based on worst case emission events supplied by consortium members. Although, two consortium member reported lower emission days (2 and 30), these were for a proportionately low tonnage and were not considered representative.
Default Release to Air	ERC 4: 95 ERC 5: 50 ERC 6B: 0.1 ERC 7: 5	%	ERC 4: 95% ERC 5: 50% ERC 6B: 0.1% ERC 7: 5%
Default Release to water	ERC 4:100 ERC 5: 50 ERC 6B: 5 ERC 7: 5	%	ERC 4:100% ERC 5: 50% ERC 6B: 5% ERC 7: 5%
Dilution factor applied for PEC derivation	10		10 (20,000 m^3/d)
Tonnage assessed	Total: 354,631 Regional: 25,000	tonnes/annum	Out of 24 combinations of uses and companies, 10 responses contained tonnage data. The total tonnage of 291276 was normalized by a factor representing the number of companies in each use to estimate the total tonnage across the industry as 354,631. Regional tonnage was taken to be the largest individual reported volume.

Table 69 Predicted Releases to the Environment Tier 1

ERC	Compartments	Predicted releases	Measured release	Explanation / source of measured data
4	Release to air	7.15 x 10^4 kg/day	-	Predicted values are those calculated by EUSES using the tonnage data and defaults for ERC4.
	Release to wastewater	7.52 X 10^4 kg/day	-	Predicted values are those calculated by EUSES using the tonnage data and defaults for ERC4.
	Soil (direct only) Agricultural soil	NA	-	No direct loss to soil is expected for this ERC.
5	Release to air	3.76 X 10^4 kg/day	-	Predicted values are those calculated by EUSES using the tonnage data and defaults for ERC5.
	Release to wastewater	3.76 X 10^4 kg/day	-	Predicted values are those calculated by EUSES using the tonnage data and defaults for ERC5.
	Soil (direct only) Agricultural soil	NA	-	No direct loss to soil is expected for this ERC.
6B	Release to air	75.2 kg/day	-	Predicted values are those calculated by EUSES using the tonnage data and defaults for ERC6B.
	Release to wastewater	3760 kg/day	-	Predicted values are those calculated by EUSES using the tonnage data and defaults for ERC6B.
	Soil (direct only) Agricultural soil	NA	-	No direct loss to soil is expected for this ERC.
7	Release to air	3760 kg/day	-	Predicted values are those calculated by EUSES using the tonnage data and defaults for ERC7.
	Release to wastewater	3760 kg/day	-	Predicted values are those calculated by EUSES using the tonnage data and defaults for ERC7.
	Soil (direct only) Agricultural soil	NA	-	No direct loss to soil is expected for this ERC.

**The predicted releases were estimated using the EUSES 2.1 program.*

In reality removal of ammonia in sewage treatment plants is highly efficient being removed first by nitrification to nitrate followed by denitrification resulting in the release of nitrogen gas. Complete consumption within the STP can be assumed and this has been used in the tier 2 assessment within EUSES

Table 70: RMMs and measured values for tier 2 assessment.

Description of RMM	Details	Effect taken into account in EUSES	Comments
Efficient removal of ammonia in STP.	0 mg/L (Local) 0 kg/d (Regional)	Lowering of calculated concentration in STP effluent. Applied at both a local and a regional level. All regional emissions to STP.	

Table 71 Predicted Releases to the Environment Tier 2

ERC	Compartments	Predicted releases	Measured release	Explanation / source of measured data
4	Release to air	7.15×10^4 kg/day	-	Predicted values are those calculated by EUSES using the tonnage data and defaults for ERC4.
	Release to wastewater	7.52×10^4 kg/day	-	Predicted values are those calculated by EUSES using the tonnage data and defaults for ERC4.
	Soil (direct only) Agricultural soil	NA	-	No direct loss to soil is expected for this ERC.
5	Release to air	3.76×10^4 kg/day	-	Predicted values are those calculated by EUSES using the tonnage data and defaults for ERC5.
	Release to wastewater	3.76×10^4 kg/day	-	Predicted values are those calculated by EUSES using the tonnage data and defaults for ERC5.
	Soil (direct only) Agricultural soil	NA	-	No direct loss to soil is expected for this ERC.
6B	Release to air	75.2 kg/day	-	Predicted values are those calculated by EUSES using the tonnage data and defaults for ERC6B.
	Release to wastewater	3760 kg/day	-	Predicted values are those calculated by EUSES using the tonnage data and defaults for ERC6B.
	Soil (direct only) Agricultural soil	NA	-	No direct loss to soil is expected for this ERC.
7	Release to air	3760 kg/day	-	Predicted values are those calculated by EUSES using the tonnage data and defaults for ERC7.
	Release to wastewater	3760 kg/day	-	Predicted values are those calculated by EUSES using the tonnage data and defaults for ERC7.
	Soil (direct only) Agricultural soil	NA	-	No direct loss to soil is expected for this ERC.

1.4.2.4.2 Exposure concentration in sewage treatment plants (STP)

Table 72: Tier 1 Concentrations in sewage

ERC for Compartment:	Estimated exposure concentrations		Measured exposure concentrations		Explanation / source of measured data
	value	unit	value	unit	
Waste water before treatment ERC 4	3.76 x 10^4	mg/L	NA	mg/L	
ERC 4 Sewage (STP effluent)	4680	mg/L	NA	mg/L	
ERC 4 Local freshwater	468	mg/L	NA	mg/L	10-fold dilution by receiving waters
Waste water before treatment ERC 5	1.88 x 10^4	mg/L	NA	mg/L	
ERC 5 Sewage (STP effluent)	2340	mg/L	NA	mg/L	
ERC 5 Local freshwater	234	mg/L	NA	mg/L	10-fold dilution by receiving waters
Waste water before treatment ERC 6B	1880	mg/L	NA	mg/L	
ERC 6B Sewage (STP effluent)	234	mg/L	NA	mg/L	
ERC 6B Local freshwater	23.4	mg/L	NA	mg/L	10-fold dilution by receiving waters
Waste water before treatment ERC 7	1880	mg/L	NA	mg/L	
ERC 7 Sewage (STP effluent)	234	mg/L	NA	mg/L	
ERC 7 Local freshwater	23.4	mg/L	NA	mg/L	10-fold dilution by receiving waters

Table 73: Tier 2 Concentrations in sewage

ERC for Compartment:	Estimated exposure concentrations		Measured exposure concentrations		Explanation / source of measured data
	value	unit	value	unit	
Waste water before treatment ERC 4	3.76 x 10^4	mg/L	NA	mg/L	
ERC 4 Sewage (STP effluent)	0	mg/L	NA	mg/L	Based on efficient removal by STP
ERC 4 Local freshwater	0	mg/L	NA	mg/L	10-fold dilution by receiving waters
Waste water before treatment ERC 5	1.88 x 10^4	mg/L	NA	mg/L	
ERC 5 Sewage (STP effluent)	0	mg/L	NA	mg/L	Based on efficient removal by STP
ERC 5 Local freshwater	0	mg/L	NA	mg/L	10-fold dilution by receiving waters
Waste water before treatment ERC 6B	1880	mg/L	NA	mg/L	
ERC 6B Sewage (STP effluent)	0	mg/L	NA	mg/L	Based on efficient removal by STP
ERC 6B Local freshwater	0	mg/L	NA	mg/L	10-fold dilution by receiving waters
Waste water before treatment ERC 7	1880	mg/L	NA	mg/L	
ERC 7 Sewage (STP effluent)	0	mg/L	NA	mg/L	Based on efficient removal by STP
ERC 7 Local freshwater	0	mg/L	NA	mg/L	10-fold dilution by receiving waters

Table 74: General emission fractions from the municipal STP

Fraction description	Fraction amount	
	value	unit
Fraction of emission directed to air by STP	0.583	%
Fraction of emission directed to water by STP	12.4	%
Fraction of emission directed to sludge by STP	0.13	%
Fraction of emission degraded by STP	86.8	%

1.4.2.4.3 Exposure concentration in aquatic pelagic compartment

Table 75: Tier 1 Local concentrations in aquatic compartment

Compartments	Local concentration aquatic (local mg/L)	Justification
ERC4 Freshwater (in mg/L)	468	
ERC4 Marine water (in mg/L)	46.8	10-fold dilution by receiving waters
ERC5 Freshwater (in mg/L)	234	
ERC5 Marine water (in mg/L)	23.4	10-fold dilution by receiving waters
ERC6B Freshwater (in mg/L)	23.4	
ERC6B Marine water (in mg/L)	2.34	10-fold dilution by receiving waters
ERC7 Freshwater (in mg/L)	23.4	
ERC7 Marine water (in mg/L)	2.34	10-fold dilution by receiving waters

Table 76: Tier 1 Predicted Environmental Concentrations (PEC) in aquatic compartment

Compartments	PEC aquatic (local mg/L)	Justification
ERC4 Freshwater (in mg/L)	468	
ERC4 Marine water (in mg/L)	46.8	
ERC5 Freshwater (in mg/L)	234	
ERC5 Marine water (in mg/L)	23.4	
ERC6B Freshwater (in mg/L)	23.4	
ERC6B Marine water (in mg/L)	2.34	
ERC7 Freshwater (in mg/L)	23.4	
ERC7 Marine water (in mg/L)	2.34	

Table 77: Tier 2 Local concentrations in aquatic compartment

Compartments	Local concentration aquatic (local mg/L)	Justification
ERC4 Freshwater (in mg/L)	0	
ERC4 Marine water (in mg/L)	0	10-fold dilution by receiving waters
ERC5 Freshwater (in mg/L)	0	
ERC5 Marine water (in mg/L)	0	10-fold dilution by receiving waters
ERC6B Freshwater (in mg/L)	0	
ERC6B Marine water (in mg/L)	0	10-fold dilution by receiving waters
ERC7 Freshwater (in mg/L)	0	
ERC7 Marine water (in mg/L)	0	10-fold dilution by receiving waters

Table 78: Tier 2 Predicted Environmental Concentrations (PEC) in aquatic compartment

Compartments	PEC aquatic (local mg/L)	Justification
ERC4 Freshwater (in mg/L)	2.82×10^{-3}	
ERC4 Marine water (in mg/L)	6.06×10^{-4}	
ERC5 Freshwater (in mg/L)	1.46×10^{-3}	
ERC5 Marine water (in mg/L)	3.17×10^{-4}	
ERC6B Freshwater (in mg/L)	4.54×10^{-5}	
ERC6B Marine water (in mg/L)	5.19×10^{-6}	
ERC7 Freshwater (in mg/L)	1.46×10^{-4}	
ERC7 Marine water (in mg/L)	3.17×10^{-5}	

1.4.2.4.4 Exposure concentration in sediments

Table 79: Tier 1 Predicted Environmental Concentrations (PEC) in aquatic sediment compartment

Compartments	PEC aquatic (local)
ERC4 Freshwater sediment (in mg/kg)	507
ERC4 Marine sediment (in mg/kg)	50.7
ERC5 Freshwater sediment (in mg/kg)	253
ERC5 Marine sediment (in mg/kg)	25.3
ERC6B Freshwater sediment (in mg/kg)	25.3
ERC6B Marine sediment (in mg/kg)	2.53
ERC6D Freshwater sediment (in mg/kg)	0.026
ERC6D Marine sediment (in mg/kg)	0.00274
ERC7 Freshwater sediment (in mg/kg)	25.3
ERC7 Marine sediment (in mg/kg)	2.53

Table 80: Tier 2 Predicted Environmental Concentrations (PEC) in aquatic sediment compartment

Compartments	PEC aquatic (local)
ERC4 Freshwater sediment (in mg/kg)	3.05×10^{-3}
ERC4 Marine sediment (in mg/kg)	6.56×10^{-4}
ERC5 Freshwater sediment (in mg/kg)	1.58×10^{-3}
ERC5 Marine sediment (in mg/kg)	3.43×10^{-4}
ERC6B Freshwater sediment (in mg/kg)	4.91×10^{-5}
ERC6B Marine sediment (in mg/kg)	5.62×10^{-6}
ERC7 Freshwater sediment (in mg/kg)	1.58×10^{-4}
ERC7 Marine sediment (in mg/kg)	3.43×10^{-5}

1.4.2.4.5 Exposure concentrations in soil and groundwater

Upon contact with soil, ammonia will be rapidly converted by a variety of bacteria, actinomycetes and fungi to ammonium (NH_4^+) by the process of ammonification or mineralization. Ammonium is then rapidly converted to nitrate. Nitrate is subsequently taken up and utilised by plants or returned to the atmosphere following denitrification; the metabolic reduction of nitrate into nitrogen or nitrous oxide (N2O) gas. The most likely fate of ammonium ions in soils is conversion to nitrates by nitrification. Therefore accumulation of concentrations of ammonia in soil and groundwater will not be expected.

1.4.2.4.6 Atmospheric compartment

Table 81: Tier 1 local concentrations in air

ERC		Estimated local exposure concentrations	Explanation / source of data
4	During emission (mg/m3)	19.9	Estimated using EUSES 2.1
	Annual average (mg/m3)	18	Estimated using EUSES 2.1
	Annual deposition (mg/m²/d)	26	Estimated using EUSES 2.1
5	During emission (mg/m3)	10.5	Estimated using EUSES 2.1
	Annual average (mg/m3)	9.45	Estimated using EUSES 2.1
	Annual deposition (mg/m²/d)	13.7	Estimated using EUSES 2.1
6B	During emission (mg/m3)	0.0209	Estimated using EUSES 2.1
	Annual average (mg/m3)	0.0189	Estimated using EUSES 2.1
	Annual deposition (mg/m²/d)	0.0351	Estimated using EUSES 2.1
7	During emission (mg/m3)	1.05	Estimated using EUSES 2.1
	Annual average (mg/m3)	0.945	Estimated using EUSES 2.1
	Annual deposition (mg/m²/d)	1.37	Estimated using EUSES 2.1

Table 82: Tier 1 Predicted Exposure Concentration (PEC) in air

ERC		Local concentration	PEC air (local+regional)	Justification
4	Annual average PEC in air, total (mg/m3)	18	18	Estimated using EUSES 2.1.
5	Annual average PEC in air, total (mg/m3)	9.45	9.45	Estimated using EUSES 2.1.
6B	Annual average PEC in air, total (mg/m3)	0.0189	0.0189	Estimated using EUSES 2.1.
6D	Annual average PEC in air, total (mg/m3)	6.62	6.62	Estimated using EUSES 2.1.
7	Annual average PEC in air, total (mg/m3)	0.945	0.945	Estimated using EUSES 2.1.

Table 83: Tier 2 local concentrations in air

ERC		Estimated local exposure concentrations	Explanation / source of data
4	During emission (mg/m3)	19.9	Estimated using EUSES 2.1
	Annual average (mg/m3)	18	Estimated using EUSES 2.1
	Annual deposition (mg/m²/d)	26	Estimated using EUSES 2.1
5	During emission (mg/m3)	10.5	Estimated using EUSES 2.1
	Annual average (mg/m3)	9.45	Estimated using EUSES 2.1
	Annual deposition (mg/m²/d)	13.7	Estimated using EUSES 2.1
6B	During emission (mg/m3)	0.0209	Estimated using EUSES 2.1
	Annual average (mg/m3)	0.0189	Estimated using EUSES 2.1
	Annual deposition (mg/m²/d)	0.0351	Estimated using EUSES 2.1
7	During emission (mg/m3)	1.05	Estimated using EUSES 2.1
	Annual average (mg/m3)	0.945	Estimated using EUSES 2.1
	Annual deposition (mg/m²/d)	1.37	Estimated using EUSES 2.1

Table 84: Tier 2 Predicted Exposure Concentration (PEC) in air

ERC		Local concentration	PEC air (local+regional)	Justification
4	Annual average PEC in air, total (mg/m3)	18	18	Estimated using EUSES 2.1.
5	Annual average PEC in air, total (mg/m3)	9.45	9.45	Estimated using EUSES 2.1.
6B	Annual average PEC in air, total (mg/m3)	0.0189	0.0189	Estimated using EUSES 2.1.
7	Annual average PEC in air, total (mg/m3)	0.945	0.945	Estimated using EUSES 2.1.

1.4.2.4.7 Exposure concentration relevant for the food chain (Secondary poisoning)

In terms of secondary poisoning, there is no evidence that ammonia bioaccumulates as the log Kow value is 0.23. Since the trigger of BCF >100 (log Kow>3) is not met, the derivation of PNECs to protect against secondary poisoning is not required. Risk characterisation ratios cannot therefore be derived.

1.4.2.4.8 Regional exposure levels and environmental concentrations.

Anhydrous ammonia is produced and used at many sites throughout a region and this may lead to a degree of regional exposure. Regional exposure has been modelled for this exposure scenario using the regional module of EUSES 2.1.

Table 85: Tier 1 regional concentrations in the environment

	Predicted regional Exposure Concentrations		Measured regional exposure concentrations		Explanation / source of measured data
	PEC value	unit	Measured value	unit	
ERC 4 Freshwater	5.72×10^{-2}	mg/L	NA	mg/L	
ERC 4 Marine water	5.34×10^{-3}	mg/L	NA	mg/L	
ERC 4 Freshwater sediments	5.47×10^{-2}	mg/kg	NA	mg/kg	
ERC 4 Marine sediments	5.12×10^{-3}	mg/kg	NA	mg/kg	
ERC 4 Agricultural soil	1.21×10^{-3}	mg/kg	NA	mg/kg	
ERC 4 Grassland	1.55×10^{-3}	mg/kg	NA	mg/kg	
ERC 4 Air	2.36×10^{-3}	mg/m^3	NA	mg/m^3	
ERC 5 Freshwater	2.88×10^{-2}	mg/L	NA	mg/L	
ERC 5 Marine water	2.68×10^{-3}	mg/L	NA	mg/L	
ERC 5 Freshwater sediments	2.74×10^{-2}	mg/kg	NA	mg/kg	
ERC 5 Marine sediments	2.57×10^{-3}	mg/kg	NA	mg/kg	
ERC 5 Agricultural soil	6.25×10^{-4}	mg/kg	NA	mg/kg	
ERC 5 Grassland	8.10×10^{-4}	mg/kg	NA	mg/kg	
ERC 5 Air	1.23×10^{-3}	mg/m^3	NA	mg/m^3	
ERC 6b Freshwater	2.78×10^{-3}	mg/L	NA	mg/L	
ERC 6b Marine water	2.42×10^{-4}	mg/L	NA	mg/L	
ERC 6b Freshwater sediments	2.64×10^{-3}	mg/kg	NA	mg/kg	
ERC 6b Marine sediments	2.32×10^{-4}	mg/kg	NA	mg/kg	
ERC 6b Agricultural soil	2.24×10^{-5}	mg/kg	NA	mg/kg	
ERC 6b Grassland	1.33×10^{-5}	mg/kg	NA	mg/kg	
ERC 6b Air	2.02×10^{-5}	mg/m^3	NA	mg/m^3	
ERC 7 Freshwater	2.88×10^{-3}	mg/L	NA	mg/L	
ERC 7 Marine water	2.68×10^{-3}	mg/L	NA	mg/L	
ERC 7 Freshwater sediments	2.74×10^{-3}	mg/kg	NA	mg/kg	
ERC 7 Marine sediments	2.57×10^{-4}	mg/kg	NA	mg/kg	
ERC 7 Agricultural soil	6.25×10^{-5}	mg/kg	NA	mg/kg	
ERC 7 Grassland	8.10×10^{-5}	mg/kg	NA	mg/kg	
ERC 7 Air	1.23×10^{-4}	mg/m3	NA	mg/m3	

Table 86: Tier 2 regional concentrations in the environment

	Predicted regional Exposure Concentrations		Measured regional exposure concentrations		Explanation / source of measured data
	PEC value	unit	Measured value	unit	
ERC 4 Freshwater	2.82×10^{-3}	mg/L	NA	mg/L	
ERC 4 Marine water	6.06×10^{-4}	mg/L	NA	mg/L	
ERC 4 Freshwater sediments	2.68×10^{-3}	mg/kg	NA	mg/kg	
ERC 4 Marine sediments	5.82×10^{-4}	mg/kg	NA	mg/kg	
ERC 4 Agricultural soil	1.18×10^{-3}	mg/kg	NA	mg/kg	
ERC 4 Grassland	1.37×10^{-3}	mg/kg	NA	mg/kg	
ERC 4 Air	2.09×10^{-3}	mg/m^3	NA	mg/m^3	
ERC 5 Freshwater	1.46×10^{-3}	mg/L	NA	mg/L	
ERC 5 Marine water	3.17×10^{-4}	mg/L	NA	mg/L	
ERC 5 Freshwater sediments	1.39×10^{-3}	mg/kg	NA	mg/kg	
ERC 5 Marine sediments	3.04×10^{-4}	mg/kg	NA	mg/kg	
ERC 5 Agricultural soil	6.09×10^{-4}	mg/kg	NA	mg/kg	
ERC 5 Grassland	7.21×10^{-4}	mg/kg	NA	mg/kg	
ERC 5 Air	1.10×10^{-3}	mg/m^3	NA	mg/m^3	
ERC 6b Freshwater	4.54×10^{-5}	mg/L	NA	mg/L	
ERC 6b Marine water	5.19×10^{-6}	mg/L	NA	mg/L	
ERC 6b Freshwater sediments	4.32×10^{-5}	mg/kg	NA	mg/kg	
ERC 6b Marine sediments	4.98×10^{-6}	mg/kg	NA	mg/kg	
ERC 6b Agricultural soil	2.08×10^{-5}	mg/kg	NA	mg/kg	
ERC 6b Grassland	4.37×10^{-6}	mg/kg	NA	mg/kg	
ERC 6b Air	6.66×10^{-6}	mg/m^3	NA	mg/m^3	
ERC 7 Freshwater	1.46×10^{-4}	mg/L	NA	mg/L	
ERC 7 Marine water	3.17×10^{-5}	mg/L	NA	mg/L	
ERC 7 Freshwater sediments	1.39×10^{-4}	mg/kg	NA	mg/kg	
ERC 7 Marine sediments	3.04×10^{-5}	mg/kg	NA	mg/kg	
ERC 7 Agricultural soil	6.09×10^{-5}	mg/kg	NA	mg/kg	
ERC 7 Grassland	7.21×10^{-5}	mg/kg	NA	mg/kg	
ERC 7 Air	1.10×10^{-4}	mg/m3	NA	mg/m3	

1.5 Exposure Scenario 5: Wide dispersive end-use: Professional uses of anhydrous and aqueous ammonia

1.5.1 Exposure scenario

Anhydrous liquid ammonia (>99.5 % wt) and aqueous ammonia solution (5-25% wt) are used by professional workers in a broad number of applications. Common applications include: use as a laboratory chemical, a refrigerant in cooling systems, a water treatment chemical, a fertiliser, a coating, paint thinner or paint remover, a photochemical, a cleaning product, a leather or other surface treatment product, a pH regulator or neutralisation agent and a process aid for nutrition.

Typical activities associated with the professional uses of ammonia where exposures can arise include operating equipment containing ammonia (e.g. opening and closing valves), transferring ammonia from storage containers using pipe or hoses, maintaining equipment and applying ammonia-based products (e.g. fertiliser, cleaning or surface treatment products).

1.5.1.1 Operational conditions related to frequency and duration of use

Operational conditions pertaining to the broad range of professional end-use scenarios involving anhydrous and aqueous forms of ammonia vary considerably across applications. A full characterisation of the frequency and duration of tasks is therefore beyond the scope of this report. For the purposes of worker exposure estimation, operational conditions have been represented generically based on the assumption that tasks may be either 1-4 hours or >4 hours in duration and that processes may be carried out either outdoors, indoors without LEV or indoors with LEV.

1.5.1.2 Risk management measures

Activities involving the use of ammonia by professionals can be regarded as wide dispersive uses: e.g. activities which deliver uncontrolled exposures. Professional workers are expected to follow good occupational hygiene practices and apply appropriate exposure control measures to minimise the potential for exposure. Workers should be trained in procedures involving the handling, sampling and transfer of ammonia and in the use of appropriate protective equipment. A good standard of general or controlled ventilation should be applied. Personal protective clothing (e.g. face/eye protection, helmet, gloves, boots and protective overalls) should be worn when any potential contact may arise. Any professional working directly with anhydrous ammonia as required to wear eye, face and respiratory protection.

1.5.2 Exposure estimation

1.5.2.1 Workers exposure

The assessment of worker exposure to anhydrous and aqueous ammonia during professional uses (ES 5) was carried out for process categories relevant to this scenario as identified by PROC codes: use and storage of ammonia in closed systems with no likelihood of exposure (PROC 1), use in closed, continuous processes with occasional controlled exposure (PROC 2), formulation using closed batch processes (PROC 3), use in batch or other processes (PROC 4), mixing or blending in a batch process (PROC 5), maintenance and clean-down (PROC 8a), transfer (PROC 8b), transfer of ammonia into containers (PROC 9), brush and roller applications (PROC 10), spraying (PROC 11), treatment of articles by dipping and pouring (PROC 13), and analysis of samples (PROC 15), hand-mixing (PROC 19) and heat and pressure transfer in closed systems (PROC 20).

A screening-level (Tier 1) assessment of worker exposure was carried out using the ECETOC Targeted Risk Assessment (TRA) model. The ECETOC TRA was used to predict dermal exposures (expressed as a daily systemic dose in mg/kg bw) and inhalation exposure concentrations (expressed as an airborne concentration in mg/m^3) associated with each process defined by PROC codes.

Exposure to workers was assessed taking into account different operational conditions that may be associated with the professional use of ammonia and the impact of different exposure control measures. Exposures were determined for task durations of 1- 4 hours or >4 hours and assuming that process are carried out either outdoors, indoors without use of local exhaust ventilation (LEV) or indoors with the use of LEV. To reflect the use of personal protective equipment (PPE), dermal exposures were determined assuming either no gloves or gloves affording 90% protection of the hands are worn. To reflect the use of respiratory protective equipment (RPE), inhalation exposures concentrations were determined assuming either no RPE or RPE affording 95% protection is worn.

The ECETOC TRA model uses a simple algorithm to determine dermal exposures that does not take the physical-chemical properties of a substance into account. The same dermal exposures where therefore predicted for anhydrous and aqueous forms of ammonia. Parameters used in the ECETOC TRA model to assess inhalation exposures were: molecular weight (35 $g.mol^{-1}$ and 17 $g.mol^{-1}$ for aqueous and anhydrous forms respectively and vapour pressure (the vapour pressure of anhydrous forms of ammonia is 8.6 x 10^5 Pa at 20°C, whereas the vapour pressure of aqueous ammonia solution between 5 and 25% w/w ranges from 5 x 10^3 Pa to 4 x10^4 Pa at 20°C. Systemic dermal exposures have been determined for a worker with bodyweight 70 kg.

1.5.2.1.1 Acute/Short term and long exposure

Potential systemic dermal exposures and inhalation exposure concentrations predicted by the ECETOC TRA model for processes associated with the professional use of ammonia are shown in Tables 87 and 88 respectively. ECETOC predicts a daily systemic dose following dermal exposure and a typical daily inhalation exposure concentration and does not specifically predict acute (short-term) and chronic (long-term) exposures. In the risk characterisation, dermal and inhalation exposures predicted by ECETOC are compared with acute and chronic DNELs values for local and systemic effects to determine the potential risk to human health associated with ES 5.

Table 87: Dermal exposures to anhydrous or aqueous (in preparations of 5-25 % w/w) ammonia predicted using the ECETOC TRA model for professional workers (ES 5)

Description of activity	PROC	Exposure assumptions		Estimated Exposure Concentration mg/kg bw/d	
		Duration	Use of ventilation	No gloves worn	Gloves worn (90% reduction)
Used in a closed process, no likelihood of exposure	PROC 1	1-4 hrs or >4 hrs	Outdoors /Indoors without LEV	0.34	0.03
Use of ammonia in a closed, continuous process with occasional controlled exposure (e.g. sampling)	PROC 2	1-4 hrs or >4 hrs	Outdoors /Indoors without LEV	1.37	0.14
		1-4 hrs or >4 hrs	Indoors with LEV	0.14	0.01
Use of ammonia in closed batch process (synthesis or formulation)	PROC 3	1-4 hrs or >4 hrs	Outdoors / Indoors without LEV	0.34	0.03
		1-4 hrs or >4 hrs	Indoors with LEV	0.03	<0.01
Use of ammonia in batch process (synthesis) where opportunity for exposure arises	PROC 4	1-4 hrs or >4 hrs	Outdoors / Indoors without LEV	6.86	0.69
		1-4 hrs or >4 hrs	Indoors with LEV	0.69	0.07
Mixing or blending in batch process	PROC 5	1-4 hrs or >4 hrs	Outdoors / Indoors without LEV	13.71	1.37
		1-4 hrs or >4 hrs	Indoors with LEV	0.07	0.01

Description of activity	PROC	Exposure assumptions		Estimated Exposure Concentration mg/kg bw/d	
		Duration	Use of ventilation	No gloves worn	Gloves worn (90% reduction)
Transfer of ammonia (charging/discharging) from/to vessels or large containers at non-dedicated facilities	PROC 8a	1-4 hrs or >4 hrs	Outdoors / Indoors without LEV	13.71	1.37
		1-4 hrs or >4 hrs	Indoors with LEV	0.14	0.01
Transfer of ammonia (charging/discharging) from/to vessels or large containers at dedicated facilities	PROC 8b	1-4 hrs or >4 hrs	Outdoors / Indoors without LEV	6.86	0.69
		1-4 hrs or >4 hrs	Indoors with LEV	0.69	0.07
Transfer of ammonia into small containers	PROC 9	1-4 hrs or >4 hrs	Outdoors / Indoors without LEV	6.86	0.69
		1-4 hrs or >4 hrs	Indoors with LEV	0.69	0.07
Roller application or brushing	PROC 10	1-4 hrs or >4 hrs	Outdoors / Indoors without LEV	27.43	0.14
		1-4 hrs or >4 hrs	Indoors with LEV	1.37	10.71
Non industrial spraying	PROC 11	1-4 hrs or >4 hrs	Outdoors / Indoors without LEV	107	10.71
		1-4 hrs or >4 hrs	Indoors with LEV	2.14	0.21
Treatment of articles by dipping and pouring	PROC 13	1-4 hrs or >4 hrs	Outdoors / Indoors without LEV	13.71	1.37
		1-4 hrs or >4 hrs	Indoors with LEV	0.69	0.07
Use as a laboratory agent	PROC 15	1-4 hrs or >4 hrs	Outdoors / Indoors without LEV	0.34	0.03
		1-4 hrs or >4 hrs	Indoors with LEV	0.03	<0.01
Hand-mixing with intimate contact and PPE only	PROC 19	1-4 hrs or >4 hrs	Indoors with LEV	141.73	14.14
Heat and pressure transfer fluids in dispersive use but closed systems	PROC 20	1-4 hrs or >4 hrs	Outdoors / Indoors without LEV	1.71	0.17
		1-4 hrs or >4 hrs	Indoors with LEV	0.14	0.01

Table 88: Inhalation exposure concentrations for anhydrous and aqueous ammonia (in preparations of 5-25 % w/w) predicted using the ECETOC TRA model for professional workers (ES 5)

Description of activity	PROC	Exposure assumptions		Anhydrous ammonia		Aqueous ammonia (5-25% w/w)	
				Estimated Exposure Concentration mg/m3		Estimated Exposure Concentration mg/m3	
		Duration	Use of ventilation	No RPE	RPE (95% reduction)	No RPE	RPE (95% reduction)
Used in a closed process, no likelihood of exposure	PROC 1	1-4 hrs or >4 hrs	Outdoors	0.00	NA	0.01	0.00
		1-4 hrs or >4 hrs	Indoors without LEV	0.01	NA	0.01	0.00
Use of ammonia in a closed, continuous process with occasional controlled exposure (e.g. sampling)	PROC 2	>4hrs	Outdoors	24.79	1.24	30.63	1.53
		>4hrs	Indoors without LEV	35.42	1.77	43.75	2.19
		>4hrs	Indoors with LEV	3.53	0.18	4.38	0.22
		1-4 hrs	Outdoors	14.88	0.74	18.38	0.92
		1-4 hrs	Indoors without LEV	22.25	1.06	26.25	1.31
		1-4 hrs	Indoors with LEV	2.13	0.11	2.63	0.13
Use of ammonia in closed batch process (synthesis or formulation)	PROC 3	>4hrs	Outdoors	49.58	2.48	61.25	3.06
		>4hrs	Indoors without LEV	70.83	3.54	87.5	4.38
		>4hrs	Indoors with LEV	7.08	0.35	8.75	0.44
		1-4 hrs	Outdoors	29.75	1.49	36.75	1.84
		1-4 hrs	Indoors without LEV	42.5	2.13	52.50	2.63
		1-4 hrs	Indoors with LEV	4.25	0.21	5.25	0.26
Use of ammonia in batch process (synthesis) where opportunity for exposure arises	PROC 4	>4hrs	Outdoors	49.58	2.48	61.25	3.06
		>4hrs	Indoors without LEV	70.83	3.54	87.5	4.38
		>4hrs	Indoors with LEV	7.08	0.35	8.75	0.44
		1-4 hrs	Outdoors	29.75	1.49	36.75	1.84
		1-4 hrs	Indoors without LEV	42.5	2.13	52.5	2.63
		1-4 hrs	Indoors with LEV	4.25	0.21	5.25	0.26

Mixing or blending in batch process	PROC 5	>4hrs	Outdoors	123.96	6.20	153.13	7.66
		>4hrs	Indoors without LEV	177.08	8.85	218.75	10.94
		>4hrs	Indoors with LEV	17.71	0.89	21.88	1.09
		1-4 hrs	Outdoors	74.38	3.72	91.88	4.59
		1-4 hrs	Indoors without LEV	106.25	5.31	131.25	6.56
		1-4 hrs	Indoors with LEV	10.63	0.53	13.13	0.66
Transfer of ammonia (charging/discharging) from/to vessels or large containers at non-dedicated facilities	PROC 8a	>4hrs	Outdoors	123.96	6.20	153.13	7.66
		>4hrs	Indoors without LEV	177.08	8.85	218.75	10.94
		>4hrs	Indoors with LEV	17.71	0.89	21.88	1.09
		1-4 hrs	Outdoors	74.38	3.72	91.88	4.59
		1-4 hrs	Indoors without LEV	106.25	5.31	131.25	6.56
		1-4 hrs	Indoors with LEV	10.63	0.53	13.13	0.66
Transfer of ammonia (charging/discharging) from/to vessels or large containers at dedicated facilities	PROC 8b	>4hrs	Outdoors	74.38	3.72	91.88	4.59
		>4hrs	Indoors without LEV	106.25	5.31	131.25	6.56
		>4hrs	Indoors with LEV	3.19	0.16	3.94	0.20
		1-4 hrs	Outdoors	44.63	2.23	55.13	2.76
		1-4 hrs	Indoors without LEV	63.75	3.19	78.75	3.94
		1-4 hrs	Indoors with LEV	1.91	0.1	2.36	0.12
Transfer of ammonia into small containers	PROC 9	>4hrs	Outdoors	99.17	4.96	122.50	6.13
		>4hrs	Indoors without LEV	141.67	7.08	175.00	8.75
		>4hrs	Indoors with LEV	14.17	0.71	17.50	0.88
		1-4 hrs	Outdoors	59.50	2.98	73.50	3.68
		1-4 hrs	Indoors without LEV	85.00	4.25	105.00	5.25
		1-4 hrs	Indoors with LEV	8.5	0.43	10.50	0.53

Roller application or brushing	PROC 10	>4hrs	Outdoors	NA	NA	153.13	7.66
		>4hrs	Indoors without LEV	NA	NA	218.75	10.94
		>4hrs	Indoors with LEV	NA	NA	21.88	1.09
		1-4 hrs	Outdoors	NA	NA	91.88	4.59
		1-4 hrs	Indoors without LEV	NA	NA	131.25	6.56
		>4hrs	Outdoors	NA	NA	13.13	0.66
Non-industrial spraying	PROC 11	>4hrs	Outdoors	NA	NA	613.20	30.66
		>4hrs	Indoors without LEV	NA	NA	876.00	43.80
		>4hrs	Indoors with LEV	NA	NA	175.20	8.76
		1-4 hrs	Outdoors	NA	NA	367.92	18.40
		1-4 hrs	Indoors without LEV	NA	NA	525.60	26.28
		>4hrs	Outdoors	NA	NA	105.12	5.26
Treatment of articles by dipping and pouring	PROC 13	>4hrs	Outdoors	123.96	6.20	153.13	7.66
		>4hrs	Indoors without LEV	177.08	8.85	218.75	10.94
		>4hrs	Indoors with LEV	17.71	0.89	21.88	1.09
		1-4 hrs	Outdoors	74.38	3.72	91.88	4.59
		1-4 hrs	Indoors without LEV	106.25	5.31	131.25	6.56
		1-4 hrs	Indoors with LEV	10.63	0.53	13.13	0.66
Use as a laboratory agent	PROC 15	>4hrs	Indoors without LEV	35.42	1.77	43.75	2.19
		>4hrs	Indoors with LEV	3.54	0.18	4.38	0.22
		1-4 hrs	Indoors without LEV	21.25	1.06	26.25	1.31
		1-4 hrs	Indoors with LEV	2.13	0.11	2.63	0.13
Hand-mixing with intimate contact and PPE only	PROC 19	<4 hrs	Outdoors	NA	NA	153.13	7.66
		<4 hrs	Indoors without LEV	NA	NA	218.75	10.94
		1-4 hrs	Outdoors	NA	NA	91.88	4.59
		1-4 hrs	Indoors without LEV	NA	NA	131.25	6.56
Heat and pressure transfer fluids in dispersive use but closed systems	PROC 20	>4hrs	Outdoors	24.79	1.24	30.63	1.53
		>4hrs	Indoors without LEV	35.42	1.77	43.75	2.19
		>4hrs	Indoors with LEV	7.08	0.35	8.75	0.44
		1-4 hrs	Outdoors	14.88	0.74	18.38	0.92
		1-4 hrs	Indoors without LEV	21.25	1.06	26.25	1.31
		1-4 hrs	Indoors with LEV	4.25	0.21	5.25	0.26

1.5.2.1 General public / consumer exposure

Professional workers are expected to conduct risk assessment to ensure that members of the public are excluded from operational activities and are not inadvertently exposed to ammonia. Consumer exposure to ammonia associated with the use of aqueous-based ammonia products has been assessed in Section 1.6 (ES 6).

1.5.2.1 Indirect exposure of humans via the environment (oral)

Ammonia is ubiquitous in the environment with <30% of emissions resulting from fertiliser uses and from non-agricultural sources (ref. 'Ammonia in the UK' - DEFRA).

In addition, there is no evidence that ammonia bioaccumulates as the log Kow value is 0.23. Since the trigger of BCF >100 (log Kow>3) is not met, the derivation of PNECs to protect against secondary poisoning is not required.

The risk of indirect exposure of humans via the environment is therefore not considered.

1.5.2.2 Environmental exposure

The majority of ammonia in the environment originates from natural sources, predominantly decaying organic matter.

Wide dispersive professional uses of ammonia are diverse and widespread. The resulting environmental exposure is not expected to add significantly to already present background levels of ammonia in the environment. An additional assessment for environmental exposure for wide dispersive uses has therefore not been performed.

1.6 Exposure Scenario 6: Wide dispersive end-use: Consumer uses of aqueous ammonia

1.6.1 Exposure scenario

Consumers may be exposed to aqueous solutions of ammonia (containing up to 25 % w/w ammonia) when using a variety of products. In this section, exposures have been assessed for the consumer use of representative common products for which default data and scenarios are available (e.g. in the ECETOC TRA model or the ConsExpo 4.1 model and RIVM Factsheets). Although data are not available for other uses (e.g. inks and toners, water treatment chemicals etc) exposures arising from these uses is not expected to be any worse than for the representative products and is therefore considered to be addressed by this assessment.

Consumers may be exposed to aqueous ammonia when using a variety of common household products including Do-It-Yourself (DIY) products such as coatings, paints, thinners and removers (PC9a) and fillers, putties and plasters (PC 9b), washing and cleaning products (e.g. all-purpose liquid; PC 35), cosmetic, personal care products such as hair dyes (PC 39) and fertilisers (PC12). Aqueous ammonia (at concentrations up to 25 % w/w) is added to water-based paints and other DIY products as a stabiliser. The composition of these products typically contains 0.2 % ammonia solution (at 25 % w/w ammonia) giving a final concentration in the product of 0.05 % w/w ammonia. Cleaning products are typically aqueous solutions containing 5 -10 % ammonia and will be diluted with water prior to use. Cosmetic products such a hair dyes contain ammonia at a maximum concentration of 4 % w/w.

Primary routes of exposure for consumers using common household products containing ammonia are the dermal and inhalation routes. Consumers are not expected to ingest ammonia during the normal use of household products and oral exposures are unlikely.

Consumer exposure to ammonia will depend on a number of factors including the frequency and duration of use. DIY products are likely to be used intermittently during the year, for several consecutive days. Cleaning products are expected to be used more frequently e.g. several times per week. Consumers are likely to use hair dye products several times per year, possibly up to once/ month. The durations of product use per day are likely to vary across the applications.

1.6.2 Exposure estimation

Consumer exposure to aqueous ammonia associated with the use of common household products (e.g. DIY, cleaning and cosmetic products) was assessed using ConsExpo version 4.1 and default assumptions presented in RIVM Factsheets relevant to the scenario being assessed. Dermal exposures were assessed using either the constant rate, dermal contact with product model or the instant application model, as appropriate. Inhalation exposure concentrations were assed using either the evaporation model or the spraying model as appropriate. To assess possible worst case scenarios, it was assumed that consumers will use DIY product at least once per month. Consumer exposure from the use of cleaning products has been assessed using the default scenario in ConsExpo 4.1 for the application of an all-purpose liquid cleaner: e.g. Household ammonia (10 % w/w ammonia) is diluted 1:80 times with water to give a final concentration of 0.125 % w/w. It is assumed that consumers will use cleaning products daily. In a worst case scenario, consumers are assume to use hair dye once per month.

Consumer exposure arising from the use of fertilisers (containing up to 25% w/w ammonia) was assessed using the ECETOC TRA model and default parameters for the scenario PC12 fertilisers: lawn and garden preparations. It is assumed that amateur gardeners will apply fertilisers twice per year.

It is reasonable to assume that consumers will not always read product labels or follow advice recommended by the manufacturer. In a worst-case assessment of consumer exposure, no use of gloves or other PPE has been assumed.

Table 89 shows the dermal exposures predicted by ConsExpo for consumer uses of common household products containing aqueous ammonia. Dermal exposures are presented as: acute systemic dermal exposures reflecting the total exposure during one event and as chronic systemic exposures reflecting the exposure per event averaged over a year taking into account the use frequency. In a conservative assessment of dermal exposures, it was assumed that 100 % of the dose is absorbed dermally.

Table 89 also shows the inhalation exposure concentrations predicted by ConsExpo for consumer uses of common household products containing aqueous ammonia. Inhalation exposure concentrations are presented as acute airborne concentrations of ammonia associated with one event and as chronic exposure concentrations reflecting the concentration per event averaged over a year taking into account the use frequency.

In the risk characterisation, predicted dermal and inhalation exposures associated with the consumer uses of common household products containing ammonia in preparations up to 25 % w/w are compared with DNEL values for acute and chronic local and systemic effects as appropriate.

Table 89: Dermal exposures to aqueous ammonia and inhalation exposure concentrations predicted by ConsExpo for consumers using common household products (e.g. DIY, cleaning and cosmetic products).

Scenario	Ammonia % w/w	Use frequency	Acute systemic dermal exposure (dose /event) mg/kg bw/day 100% dermal absorption	Chronic systemic dermal exposure (dose averaged over 1 year) mg/kg bw/day 100% dermal absorption	Acute inhalation exposure concentration (1 event) mg/m3	Chronic inhalation exposure concentration (yearly average) mg/m3
PC9 Coatings, paints, thinners, removers (0.05% w/w ammonia)						
Applying waterborne paint using brush and roller	0.05	1 event /month	0.03	8.2×10^{-5}	7	0.0018
Spraying paint from a can (application)	0.05	1 event /month	0.013	6.8×10^{-5}	0.67	5.1×10^{-5}
Applying general coatings	0.05	1 event /month	0.0021	1.9×10^{-6}	6.7	2.4×10^{-4}
Applying paint remover	0.05	1 event /month	0.0042	1.1×10^{-5}	3.2	3.6×10^{-4}
PC9b Fillers, putties, plasters etc (0.05 % w/w ammonia)						
Applying filler	0.05	1 event /month	4.2×10^{-4}	3.4×10^{-6}	0.37	5.1×10^{-3}
PC35 Washing and cleaning products (0.125 % w/w ammonia)						
Applying all-purpose liquid cleaner / detergent	0.125	104 times/ year	0.41	0.12	3.3	0.16
PC39 Cosmetics, personal care products (4% w/w ammonia)						
Applying hair dye	4	1 event / month	67	2.203	NA	NA
PC12 Fertilisers: lawn and garden preparations (25 % w/w ammonia)						
Applying fertilisers	25	2 events/year	35.7		NA	NA

1.6.2.1 Environmental exposure

The majority of ammonia in the environment originates from natural sources, predominantly decaying organic matter.

Wide dispersive consumer uses of ammonia are diverse and widespread. The resulting environmental exposure is not expected to add significantly to already present background levels of ammonia in the environment. An additional assessment for environmental exposure for wide dispersive uses has therefore not been performed.

SDS EXPOSURE SCENARIO (ES)
AMMONIA (ANHYDROUS)

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