ESSEMAR S.p.A.

SAFETY DATA SHEET

In accordance with Regulation (EC) 1907/2006 (REACH), Annex II

1. IDENTIFICATION OF THE SUBSTANCE AND OF THE COMPANY		
1.1 Product identifier		
Trade name:		Oleum
Index number:		016-019-00-2
CAS number:		8014-95-7
REACH registration n:		see section 3 (it is a mmixture)
1.2 Relevant identified uses of the substance or mixture and uses advised against		
Uses: (see corresponding ES as attachement to this SDS)		Production of sulphur trioxide Use of sulphur trioxide as an intermediate Use of oleum as a nitration agent Formulation of oleum
Uses advised against:		None known
1.3 Details of the supplier of the safety data sheet		
Manufacturer/Importer/Supplier:		**ESSEMAR Spa** – Via San Cassiano 99 – 28069 San Martino di Trecate (NO) Tel +39 03217901, fax +39 0321779646
Person responsible for the Safety Data Sheet (with e-mail address)		laboratorio@marchi-industriale.it
1.4 Emergency telephone number		
Emergency phone number (Poison centre H24)		Milano – 0266101029 / Napoli – 0817472870 Pavia – 038224444 / Bergamo - 035269469 Roma – 063054343 opp. 06490663
2. HAZARDS IDENTIFICATION		
2.1 Classification of the substance		
Classification in accordance with Regulation 1272/2008 (CLP)		
Hazard statement(s):	H314: Skin Corr. 1A H335 STOT Single Exp. 3	Causes severe skin burns and eye damage May cause respiratory irritation

Classification in accordance with Directive 67/548 (DSD)		
Risk phrase(s):	C; R35 Xi, Irritating R37 R14	Corrosive, Causes severe burns Irritating to respiratory system reacts violently with water
2.1.3 Additional information	Risk advice to man and the environment Fuming acid forms acidic mists. Both the mist and the solution have a corrosive effect on human tissue. Environmental effects might occur on a local scale by pH effects.	
2.2 Label elements		
Labelling in accordance with Regulation 1272/2008 (CLP)		
Hazard pictogram:		
Signal word		Danger
Hazard statement(s):	H314 H335 EUH014	Causes severe skin burns and eye damage May cause respiratory irritation Reacts violently with water
Precautionary statement(s):	P260: Do not breathe dust/fume/gas/mist/vapours/spray. P264 Wash hands thoroughly after handling P280 Wear protective gloves/protective clothing/eye protection/face protection. P301+P330+P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting. P305+P351+P338: IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. P303+P361+P353: IF ON SKIN (or hair): Remove/Take off immediately all contaminated clothing. Rinse skin with water/shower. P304+P340: IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing. P403+P233: Store in a well-ventilated place. Keep container tightly closed. P312: Call a POISON CENTER or doctor/physician if you feel unwell. P405 Store locked up. P501: Dispose of contents/container to permited recycling or waste destruction company	
In case of a mixture: Labelling in accordance with 1999/45 (DPD)		
Hazard symbol(s):		

Contains:		Sulphur trioxide
Risk phrase(s):	C; R35 Xi, Irritating R37 R14	Corrosive, Causes severe burns Irritating to respiratory system reacts violently with water

2.3 Other hazards

PBT/vPvB criteria:	According to Annex XIII of Regulation (EC) No 1907/2006, no PBT and vPvB assessment has been conducted since the substance is inorganic.
Other hazards:	None known.

3. COMPOSITION/INFORMATION ON INGREDIENTS

Substances

According to the REACH Regulation the product is a mixture.

Chemical name (Registration number)	CAS no.	EC no.	IUPAC name	Purity
Sulphur trioxide (01-2119458835-26-0029)	7446-11-9	231-197-3	Oxosulfane dioxide	20-30%
Sulfuric acid (01-2119458838-20-0105)	7664-93-9	231-639-5	sulfuric acid	70-80%

4. FIRST-AID MEASURES

4.1 Description of first aid measures

Eye contact:	Immediately wash eyes with plenty of running water for at least 15 minutes, occasionally lifting the upper and lower eyelids. Remove contact lenses, if present and easy to do. Seek medical advice if irritation develops and persists.
Skin contact:	Wash affected skin area with plenty of water and soap for at least 15 minutes thoroughly while removing contaminated clothing and shoes. Seek medical advice if irritation develops and persists.
Ingestion:	Seek medical advice if the victim feels unwell. Wash out mouth with plenty of water and give plenty of water to drink. Do not induce vomiting. Never give anything by mouth to an unconscious person.
Inhalation:	Remove the victim from exposure into fresh air immediately if adverse effects (e.g. dizziness, drowsiness or respiratory irritation) occur. If not breathing, give artificial respiration. If breathing is difficult, give oxygen. Get medical aid. Also seek medical advice if cough or other symptoms appear. Do not use mouth-to-mouth respiration. Seek medical advice immediately when vapors are intensively inhaled.

4.2 Most important symptoms and effects

Symptoms	corrosive to the eyes, mucous membranes and exposed areas of skin.
Risks	Causes severe skin burns and eye damage

4.3 Indication of any immediate medical attention and special treatment needed
Remove/Take off immediately all contaminated clothing. Rinse skin/eyes with water/shower. Move out of dangerous area

5. FIRE-FIGHTING MEASURES

5.1 Extinguishing media

Suitable:	All media
Not suitable:	No unsuitable extinguishing media known

5.2 Special hazards arising from the substance or mixture
Product is nonflammable and does not support combustion.
Move away from container and cool with water from a protected position.
The product reacts with most metals producing explosive hydrogen gas and sulphur oxides.
The substance is readily dissociated in water into hydrated protons and sulphur ions

5.3 Advice for firefighters
In case of insufficient ventilation wear suitable respiratory equipment
Spillages or uncontrolled discharges into watercourses must be IMMEDIATELY alerted to the Environmental Agency or other appropriate regulatory body.
Absorb with inert, damp, non-combustible material, then flush area with water. Collect spillage in containers, seal securely and deliver for disposal according to local regulations.

6. ACCIDENTAL RELEASE MEASURES

6.1 Personal precautions, protective equipment and emergency procedures

For personal protection see section 8.
Use personal protective equipment.
Ensure adequate ventilation

6.2 Environmental precautions

Spillages or uncontrolled discharges into watercourses must be IMMEDIATELY alerted to the Environmental Agency or other appropriate regulatory body.
Absorb with inert, damp, non-combustible material, then flush area with water. Collect spillage in containers, seal securely and deliver for disposal according to local regulations

6.3 Methods and material for containment and cleaning up
Neutralize large spillages with lime or soda ash. Rinse remnant with plenty of water.
Refer to section 13 for disposal of spilled material.

6.4 Reference to other sections
See section 8 for personal protective equipment and section 13 for waste disposal

7. HANDLING AND STORAGE

7.1 Precautions for safe handling

Technical measures/ Precautions:	For personal protection see section 8. The usual precautions for handling chemicals should be observed. Avoid any direct contact with the material and formation of aerosol. Do not breathe gas/fumes/ vapor/spray and avoid contact with skin and eyes. Smoking, eating and drinking should be prohibited in the application area. Product is nonflammable and does not support combustion.
General occupation hygiene:	Do not to eat, drink and smoke in work areas. Wash hands after use. Remove contaminated clothing and protective equipment before entering eating areas.

7.2 Conditions for safe storage, including any incompatibilities

Technical measures/ Storage conditions:	No smoking. Keep in a well-ventilated place. Do not store together with alkalies and oxidants. Keep container tightly closed. Store in plastic tanks Eye wash facilities and emergency shower must be available when handling this product For safety, store below: 40 °C
Incompatible products:	Use only metal containers with acid resistand innerlayers, product may be corrosive to metals.

8. EXPOSURE CONTROLS / PERSONAL PROTECTION

8.1 Control parameters

Regulated occupational exposure limit values: (derived from sulphuric acid data)

Components	CAS-No.	Value	Control parameters	Update	Form of exposure
Sulfuric acid	7664-93-9	STEL (15 min) TWA 8 hours	0,05 mg/m³ 0,1 mg/m³	recent	aerosols mist and gas
Further information	STEL and TWA for sulphuric acid are derived and are EU Indicative Occupational Exposure Limits (1994)				

Recommended occupational and consumer exposure limit values (following from the performed CSA):	DNEL: Acute inhalation exposure: the SCOEL recommends a STEL (15 min) of 0,1 mg/m³ long term inhalation exposure: the SCOEL recommends a TWA 8 hour of 0,05 mg/m³ PNEC: PNEC aqua (marine water): 0,002 mg/L PNEC aqua (freshwater): 0,0025 mg/L
8.2 Exposure controls	
Appropriate engineering controls:	Effective exhaust ventilation system Ensure that eyewash stations and safety showers are close to the workstation location. Attachd Exposure Scenarios provide a 360 days/year exposition.
Environmental exposure controls:	Dispose of rinse water in accordance with local and national regulations.
Individual protection measures, such as personal protective equipment	
Respiratory protection:	Provide extract ventilation to material transfer points and other openings. Carry out in a vented booth provided with laminar airflow. Automate activity where possible. Wear acid vapour mask (eg DIN 3181 ABEK)
Hand protection:	Wear suitable gloves tested to EN374 (e.g. PVC or rubber gloves)
Eye protection:	Use safety eyewear designed to protect against splash of liquids. Tightly fitting safety goggles.
Skin and body protection:	Protective suit, apron and boots. Choose body protection according to the amount and concentration of substance at the work place
Hygiene measures:	Handle in accordance with good industrial hygiene and safety practice. When using do not eat or drink. When using do not smoke. Wash hands before breaks and at the end of workday. Plan first aid action before beginning work with this product.
General advice Air Soil Water	Do not flush into surface water or sanitary sewer system. Do not flush into surface water or sanitary sewer system.Hose down gases, fumes and/or dust with water. Avoid subsoil penetration.Do not let product enter drains.

9. PHYSICAL AND CHEMICAL PROPERTIES	
9.1 Information on basic physical and chemical properties	
Appearance:	Colourless, liquid, fuming
Odour:	odourless
pH (20°C)	<0,3
Melting/Freezing temperature:	c.a. 16,8°C
Boiling temperature:	44,8°C (1013 hPa)
Flash-point:	Not relevant as the substance is an inorganic solid.
Flammability:	Non flammable (based on molecular structure)
Explosive properties:	Not explosive
Oxidizing properties:	Not oxidising
Vapour pressure:	Depends on forms: 97,3 – 577,2 hPa - at 25°C)
Relative density	c.a. 1922 kg/m³ (20 °C) (conc. al 100%)
Solubility in water:	Completely miscible at ca. 20 °C
Partition coefficient n-octanol/water:	Not relevant as the substance is inorganic, but considered to be low (based on high water solubility)
Viscosity:	N.A.
9.2 Other information	
10. STABILITY AND REACTIVITY	
10.1 Reactivity Stable under recommended storage and handling conditions (see section 7, handling and storage).	
10.2 Chemical stability Reaction with strong oxidising agents. Reaction with alkaline substances (bases).	
10.3 Possibility of hazardous reactions	

The product reacts with metals with evolution of highly flammable hydrogen. The acid reacts violent with alkalies with evolution of heat.

10.4 Conditions to avoid

Any use involving aerosol formation or vapor release in excess of 0,05 mg/m³ where workers are exposed without respiratory protection. Any use carrying a risk of splashes to eyes / skin where workers are exposed without eye/skin protection

10.5 Incompatible materials

Metals, oxidant, alkali, hydrochloric acid

10.6 Hazardous decomposition products

Sulphur oxides / Hydrogen.

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

The substance is a strong, highly corrosive acid. The substance only causes local effects and no systemic effects. It rapidly dissociates almost completely in contact with water, releasing the sulphur ion and the hydrogen ion which combines with water to form the hydronium ion. Both sulphur and hydronium ions are normally present in the body.

ACUTE TOXICITY	
Acute oral toxicity:	No data available
Acute dermal toxicity:	No data available
Acute inhalation toxicity:	Sulfuric acid derived data Aeresol LC_{50}: (rat) 375 mg/m^3 LC_{50} (mouse – 4 h exposition): 0,85 mg/L air LC_{50} (mouse – 8 h exposition): 0,60 mg/L air LC_{50} (rabbit – 7 h exposition): 1,61 mg/L air Vapour: LC_{50}: (rat - 2 h exposition): 0, 51 mg/L air LC_{50} (mouse – 2 h exposition): 0, 32 mg/L air
LOCAL EFFECTS	
Skin irritation:	Corrosive. Studies with results indicating corrosivity to the skin
Eye irritation:	Risk of serious damage to eyes (not reversible)

Skin sensitization:	Not sensitizing (OECD 406)
OTHER	
Repeated dose toxicity	**Oral:** No data available from repeated dose oral studies **Dermal:** No data available from repeated dose dermal studies **Inhalation:** Sub-chronic inhalation NOAEC is 150 ppm for rats/mice, 30-90-days, 12-23,5 hours/days Chronic inhalation NOAEL is 10 mg/m^3 for rats/mice, 26-weeks, 6 hours/days, 5 days/week.
Mutagenicity:	Not mutagenic, not clastogenic
Reproductive toxicity:	No data available
Carcinogenicity:	The available animal data do not support the classification of oleum for carcinogenicity
12. ECOLOGICAL INFORMATION	
12.1 Toxicity	
Read-across data with sulphuric acid. It is accepted that the aquatic toxicity of sulphuric acid results if sufficient acid is present to produce a very low pH (i. e. pH 3-5). Given that the environmental exposure assessment shows insignificant perturbation of aquatic pH levels from the formulation of the product and its proposed use, it is considered that there is no long-term risk to aquatic organisms and therefore chronic fish effects data are not required.	
Fish (short-term):	96-h LC_{50}: 16-28 mg/l (pH 3,25-3,5)
Fish (long-term):	EC10/LC10 o NOEC : 0,025 mg/L
Daphnia magna (short-term):	48-h EC_{50}: >100 mg/l (OECD 202)
Daphnia magna (long-term):	EC10/LC10 o NOEC : 0,15 mg/L
Algae:	72-h ErC_{50}: > 100 mg/l
M factor	10
Inhibition of microbial activity:	No available data
12.2 Persistence and degradability	
Biodegradation:	As the active substance, is an inorganic compound, which is not biologically degradable, the ready biodegradability, inherent biodegradability and biodegradation in seawater are scientifically impossible to perform.

	In addition, the proposed use of sulphuric acid is not expected to lead to significant releases to marine water.
Hydrolysis:	Due to its intrinsic properties, it is scientifically impossible to perform a hydrolysis test. In addition, since the behaviour of sulphuric acid in water is known, it is also not scientifically necessary
12.3 Bioaccumulative potential	
Bioconcentration factor (BCF):	No bioaccumulation expected.
12.4 Mobility in soil	
Adsorption coefficient:	Terrestrial compartment is not expected to be relevant. If emitted to soil, adsorption to soil particles will be negligible. Depending on the buffer capacity of the soil, H^+ will be neutralized in the soil pore water by natural organic or inorganic matter or the pH may decrease.
12.5 Results of PBT and vPvB assessment The substance does not fulfil all criteria to be classified as a PBT or vPvB substance **Persistence Assessment** The substance can be regarded as non biodegradable in the aquatic and terrestrial environment. The test results suggest that the substance is persistent. Therefore the criteria for the P classification are met. **Bioaccumulation Assessment** The substance is considered cationic at environmental pH levels, the log Kow was calculated to a value of -1. Following the Annex VIII Guidance this value does not impose any bioaccumulation potential	
13. DISPOSAL CONSIDERATIONS	
Waste from residues:	Do not dispose of waste into sewer. Do not contaminate ponds, waterways or ditches with chemical or used container. Hazardous waste CER code 06 01 01 Do not dispose of waste into sewer. Do not contaminate ponds, waterways or ditches with chemical or used container. All contaminated waste water must be processed in an industrial or municipal wastewater treatment plant that incorporates both primary and secondary treatments Site should have a spill plan to ensure that adequate safeguards are in place to minimize the impact of episodic released.
Container:	Empty remaining contents. Contaminated packaging According to local regulations
14. TRANSPORT INFORMATION	

ADR	**RID**
UN Number: 1831 UN proper shipping name: Fuming Sulphuric acid Transport hazard class: 8 Classification Code: CT1 Packing group: I Label: 8+6.1 Tunnel restriction code: (C1D) Hazard identification n. : X886 Environmentally hazardous: no	UN Number: 1831 UN proper shipping name: Fuming Sulphuric acid Transport hazard class: 8 Classification Code: CT1 Packing group: I Label: 8+6.1 Hazard identification n. : X886 Environmentally hazardous: no
	

15. REGULATORY INFORMATION

15.1 Safety, health and environmental regulation/legislation specific for the substance or mixture:	
15.2 Chemical safety assessment:	Chemical Safety Assessments have been carried out for these substances.

16. OTHER INFORMATION

The information provided in this safety data sheet is correct to the best of our knowledge, information, and belief at the date of its publication. The information given is designed only as guidance for safe handling, use, processing, storage, transportation, disposal, and release and is not to be considered a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any proceed, unless specified in the text.

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ANNEX

Exposure scenarios

ES1Production of sulphur trioxide
Sector of Use:
SU3: Industrial uses: Uses of substances as such or in preparation at industrial sites

Produce Category:
Not applicable

Process Categories:
PROC01: Use in closed process, no likelihood of exposure
PROC02: Use in closed, continuous process with occasional controlled exposure
PROC08b: Transfer of substance or preparation (charging/discharging) from/to vessels/large containers at dedicated facilities
PROC09: Transfer of substance or preparation into small containers (dedicated filling line, including weighing)

Environmental Release Category:
ERC01: Manufacture of Substances

Operational conditions related to frequency, duration and amount of use
The production of sulphur trioxide is generally a continuous/batch production, with the process running for long periods without interruption, for up to 360 days per year. Operators work a standard shift and normal working week, with production continuing at weekends. Planned maintenance and shutdowns occur only every few years.
Duration, frequency and amounts

Information type	Data field	Explanation
Use amount per worker [workplace] per day	No data	Worker exposure considered to be negligible due to the specialised systems and closed nature of the production process.
Duration per day at workplace [for one worker]	8hr/d	Standard number of hours in one work day
Frequency at workplace [for one worker]	220 d/y	Standard number of work days / year
Other determinants related to duration, frequency and amount of use	Intermittent contact is expected	These tasks rarely take a full 8hr / day so worst case is assumed.
Annual amount used per site	60,000 t/y	Worst case for single production site
Emission days per site	360 d/y	Estimate number of emission days, based on continuous production

Operational conditions and risk management measures related to product characteristics
Product Characteristic

Information type	Data field	Explanation
Type of product the information relates to	Substance as such or substance in oleum	The product is in liquid form in a sealed tank container in both cases.
Physical state of product	Liquid	
Concentration of substance in product	> 98 %	

Remarks or additional information:
Respiration volume and skin contact under conditions of worker uses

Information type	Data field	Explanation
Respiration volume under conditions of use	10m^3/d	Default value for a worker breathing for a 8h work day in RIP 3.2
Skin contact area with the substance under conditions of use	480cm^2 (ECETOC default)	Please note that due to the corrosive nature of sulphur trioxide and sulphuric acid dermal exposure is not considered relevant for risk characterisation as it must be prevented in all cases.

Conditions leading to dilution of initial release related to human health

Information type	Data field	Explanation
Room size and ventilation rate	NA	Not relevant as workers involved in production work in a control room, with no direct contact to the installations housing the material

Conditions leading to dilution of initial release related to environment

Information type	Data field	Explanation
Discharge volume of sewage treatment plant	2000 m^3/d	EUSES default value for standard local STP
Available river water volume to receive the emissions from a site	20,000 m^3/d	Standard ERC flow rate leading to a 10 fold dilution in receiving waters.

Risk management measures
Exhaust gasses from the incineration process can be filtered and scrubbed; typically this removes >99% of sulphur oxide gases with the outflow being continually analysed for sulphide gas content which would generally be sulphur dioxide rather than sulphur trioxide.
Workers involved in production, handing, sampling and transfer of materials are trained in the procedures and protective equipment is intended to cope with the worst case scenario, in order to minimise exposure and risks. This may include chemical resistant clothing, goggles and respiratory equipment where required. Due to the nature of the materials the level of control and system closure is extremely high and so in reality exposure is highly unlikely. Primary emission sources are not located in the breathing zone of the worker as workers are in a separate control room. The handling of sulphur trioxide is such that contact between product and adjacent air is reduced and controlled loading is used reducing the amount of aerosol formation. Vapour recovery systems and local exhaust ventilation such as enclosing hoods are used where required. Emission sources are completely segregated from the work environment by isolating the source in a fully enclosed and separate room and there is complete personal enclosure with ventilation where necessary. The processes are generally fully enclosed (air tight) and the integrity of the enclosure is monitored. The facilities are housed outdoors, not close to buildings and workers are generally located > 4 metres from far field source.
Environmental emissions are limited by designated waste treatment process designed to limit environmental exposure to all relevant compartments. Waste gas emissions are scrubbed and may also then be diverted to the wastewater stream. This significantly lessens the possible emission by atmospheric deposition to soil or surface waters. Liquid wastes would generally contain sulphuric acid that has formed when sulphur trioxide contacts water and these converted wastes are treated (neutralisation to neutral pH) prior to emission to remove any sulphuric acid in the waste water and sludge from the waste water treatment plant is sent for incineration or landfill and is not used for agricultural spreading. This precludes any contamination of soil by sludge spreading. Waste water treatment is usually carried out by neutralisation followed by flocculation or decantation.
Risk management measures for industrial site

Information type	Data field	Explanation
Containment and local exhaust ventilation		
Containment plus good work practice required	Effectiveness: Unknown	Production and handling of sulphur trioxide involves special equipment and high integrity contained systems with little or no potential for exposure. Facilities involved in the production and uses of sulphur trioxide are completely segregated from the work environment by isolating the source in a fully enclosed and separate room and there is complete personal enclosure with ventilation in situations where exposure could occur. The processes are fully enclosed (air tight) and the integrity of the enclosure is monitored. The facilities are housed outdoors, not close to buildings and workers are generally located > 4 metres from far field source.
Local exhaust ventilation is required	Effectiveness : Unknown	Vapour recovery systems and local exhaust ventilation such as enclosing hoods are used.
Personal protective equipment (PPE)		
Type of PPE (gloves, respirator, face-shield etc)	Effectiveness: Unknown	Workers involved in sampling and transfer of materials to road tankers are trained in the procedures and protective equipment is intended to cope with the worst case scenario, in order to minimise exposure and risks.
Other risk management measures related to workers		
Primary emission sources are not located in the breathing zone of the worker as workers are in a separate control room. The handling of sulphur trioxide is such that contact between product and adjacent air is reduced and submerged loading is used reducing the amount of aerosol formation.		
Risk management measures related to environmental emissions from industrial sites		
Onsite pre-treatment of waste water	Chemical pre-treatment or	Waste waters are generally treated on site by chemical neutralisation methods before release to the

Information type	Data field	Explanation
	onsite STP.	municipal STP or to the environment.
Resulting fraction of initially applied amount in waste water released from site to the external sewage system	Varies depending on system.	The neutralisation process is extremely efficient and pH monitors are in place to ensure that complete neutralisation and removal have taken place. Complete conversion of sulphur trioxide to sulphuric acid in the waste stream is expected.
Air emission abatement	Effectiveness: Adequate measures in place	Exhaust gases from the production treated by scrubbers.
Onsite waste treatment	Effectiveness: complete	The waste water neutralisation process is extremely efficient with almost total neutralisation achieved. pH alarms are in place to ensure that successful neutralisation has taken place.
Effluent (of the waste water treatment plant) discharge rate	2000 m^3/d	Default: 2.000 m^3/d
Recovery of sludge for agriculture or horticulture	No	All sludge is collected and incinerated or sent to landfill.
Resulting fraction of initially applied amount in waste water released from site	Complete removal	In the second tier removal of formed sulphuric acid by neutralization has been considered.

Workers exposure
The assessment of worker exposure to sulphur trioxide (and subsequent sulphuric acid mists in air) from production (ES1) was carried for processes relevant to this use scenario as identified by PROC codes. Initially, a screening-level (Tier 1) assessment was carried out using the ECETOC Targeted Risk Assessment (TRA) model. A higher tier (Tier 2) refinement of the Tier 1 assessment was carried out using the Advanced REACH Tool (ART).
Acute/short -term and long-term exposure
Parameters used in the ECETOC TRA model to conduct a Tier 1 assessment of inhalation exposure concentrations

	Parameter	Explanation/source of data
Molecular weight	80.06 g/mol	
Vapour Pressure	9730 Pa	
Water solubility	10000 mg/L	Representative value used in modelling as sulphur trioxide rapidly hydrolyses in water to form sulphuric acid which is highly miscible.
Is the substance a solid?	No – liquid	
Dustiness during process	n/a	Only in the case of solid
Duration of activity	>4 hours (default)	
Use of ventilation	Indoors with LEV	
Use of respiratory protection	Yes, 95% efficiency	

First tier screening level exposure concentrations to workers

Description of activity	PROC	Physical state of material	Estimated Exposure Concentrations	
			value	unit
Production (High integrity closed system, sampling via closed loop)	1	Liquid	1.67 x10^{-03}	mg/m^3
Production and sampling (Occasional exposure system)	2	Liquid	1.67 x10^{-01}	mg/m^3
Loading/transfer	8b	Liquid	2.50 x10^{-01}	mg/m^3
Loading/transfer (Small containers)	9	Liquid	8.34 x10^{-01}	mg/m^3

Parameters and assumptions used in the ART model to conduct a Tier 2 assessment of inhalation exposure concentrations

	PROC	Parameters/ assumptions
Exposure duration	All	480 min
Product type	All	Liquid
Process temperature	PROC 1,2	Hot processes (50-150°C)
	PROC 8b, 9	Room temperature (15-25°C)
Vapour pressure	All	9730 pa
Liquid weight fraction	All	Pure liquid (100%)
Primary emission source proximity	All	Primary emission source is not located in the breathing zone of the worker - the assessment for this activity involves a primary far-field emission source only (workers are in a control room)
Activity class	All	Transfer of liquid products
Containment	PROC 1,2, 9	Handling reduces contact between product and adjacent air, controlled loading
	PROC 8b	n/a due to bottom loading or tankers
Localised controls	PROC 1,8b, 9	Vapour recovery systems; LEV
	PROC 2	Vapour recovery
Segregation	PROC 1,2, 9	Complete segregation of workers in separate control room
	PROC 8b	Partial segregation of workers
Fugative emission source	PROC 1,8b,9	Process fully enclosed – not openly breached for sampling
	PROC 2	Not fully enclosed – effective housekeeping practices in place.
Dispersion	PROC 1,2	Outdoors not close to buildings, worker located >4 meters from far field source
	PROC 8b	Outdoors close to buildings, worker located >4 meters from far field source
	PROC 9	Indoors, any sized room, only good natural ventilation

Tier 2 acute/short-term and long-term inhalation exposure concentrations derived using the ART model

Description of activity	PROC	Physical state of material	Estimated Short-term Exposure Concentrations (mg/m3)		Estimated Long-term Exposure Concentration (mg/m3)	
			50th percentile value	90th percentile value	50th percentile value	90th percentile value
Production (High integrity closed system, sampling via closed loop)	1	Liquid	2.2×10^{-04}	1.5×10^{-03}	5.4×10^{-04}	1.3×10^{-03}
Production and sampling (Occasional exposure system)	2	Liquid	2.2×10^{-03}	1.5×10^{-02}	5.4×10^{-03}	1.3×10^{-02}
Loading/transfer	8b	Liquid	2.2×10^{-03}	1.5×10^{-02}	5.4×10^{-03}	1.3×10^{-02}
Loading/transfer (Small containers)	9	Liquid	1.1×10^{-02}	3.3×10^{-02}	1.3×10^{-02}	2.9×10^{-02}

Consumer exposure
Consumers are not directly exposed to sulphur trioxide during the processes associated with ES1 as this exposure scenario involves only closed industrial processes.
Indirect exposure of humans via the environment (oral)
Indirect exposure of humans via the environment is expected to be negligible. Sulphur trioxide converts to sulphuric acid upon contact with environmental moisture. This sulphuric acid is fully miscible in water and, as such, will not persist in any environmental compartment where indirect exposure of humans could occur. Furthermore none of the processes associated with sulphur trioxide production involve any targeted environmental emissions or application and the primary receiving compartment is the on-site STP where rigorous neutralisations processes and employed. Removal in the STP is expected to be efficient and so secondary exposure of the other receiving compartments is expected to be minimal. Similarly contamination of food crops or animals used as human food sources is not envisaged.
Environmental exposure
EUSES inputs for production of sulphuric acid

Input parameter:	Value:	Unit:	ERC default (if applicable)
Molecular Weight	80.06	g/mol	
Vapour Pressure (at 25 °C)	9730	hPa	
Water Solubility	1000	mg/L	

Input parameter:	Value:	Unit:	ERC default (if applicable)
Octanol/water partition coefficient	-1 (estimated)	logKow	
Koc	1 (estimated)		
Biodegradability	Not biodegradable (inorganic oxides cannot be considered biodegradable)		
Life Cycle Step	Production		
Environmental Release Class	ERC1		
Fraction of Tonnage for Region (1st Tier)			1
STP			Yes
Emission events per year	360 (manufacturer information)	Days	300
Default Release to Air	5	%	5
Default Release to water	6	%	6
Dilution factor applied for PEC derivation			10 (20,000 m^3/d)
Tonnage assessed	Local: 60,000 Regional: 350,000	tonnes/annum	Worst case local and total regional production tonnage.

For the tier 2 assessment of environmental releases the effects of several RMMs have been investigated alongside the worst case measured values obtained from consortium members to cover the production or sulphur trioxide.

RMMs and measured values for tier 2 assessment.

Description of RMM	Details	Effect taken into account in EUSES	Comments
No loss to waste water	0 mg/L	Lowering of concentration in STP effluent to 0 mg/L due to the conversion of sulphur trioxide to sulphuric acid and the very efficient neutralization process to remove sulphuric acid in the waste stream	Total neutralization to around pH 7.
Emission and production days	360 emission days per year	Increase emission days by 20%.	Continuous production
Sludge removal	Sludge removed to landfill or incinerated.	Concentration in soil due to sludge spreading set to 0.	No contamination of grassland or agricultural soil.

Predicted Releases to the Environment Tier 2

ERC	Compartments	Predicted releases	Measured release	Explanation / source of measured data
1	Aquatic freshwater (after STP)	0 kg/d	-	Based on efficient neutralization
	Release to air	8,260 kg/d	-	
	Soil (direct only) Agricultural soil	0 kg/d	-	No directly loss to soil is expected for this ERC and no sludge spreading.

ES 2: Use of sulphur trioxide as an Intermediate

Sector of Use:

SU3: Industrial uses: Uses of substances as such or in preparation at industrial sites
SU8: Manufacture of bulk, large scale chemicals (including petroleum products)
SU9: Manufacture of fine chemicals

Produce Category:

PC19: Intermediate

Process Categories:

PROC01: Use in closed process, no likelihood of exposure
PROC02: Use in closed, continuous process with occasional controlled exposure
PROC03: Use in closed batch process (synthesis or formulation)
PROC04: Use in batch and other process (synthesis) where opportunity for exposure arises
PROC08b: Transfer of substance or preparation (charging/discharging) from/to vessels/large containers at dedicated facilities
PROC09: Transfer of substance or preparation into small containers (dedicated filling line, including weighing)

Environmental Release Category:

ERC6A: Industrial use resulting in manufacture of another substance (use of intermediates)

Description of activities and processes covered in the exposure scenario

Generally intermediate use of sulphur trioxide is continuous with single site use rates ranging between 15 and around 30 tonnes per day in a large facility. The large size of the typical facility involved means that all vessels and reactors are housed out-doors, managed by a small number of operators working in a separate enclosed control room.
Because of the conditions required (such as high temperatures) in the processes (and the nature of sulphur trioxide and the produced gases) all reactors and pipelines are sealed and insulated, to prevent loss of the reaction materials and maintain the necessary temperatures, and to protect the workforce and the environment.
All processes are very highly contained. Most facilities dealing with sulphur trioxide, in all relevant process types, are large-scale outdoor plants.
Road tanker connecting and disconnecting (loading and unloading) generally takes place in the open air with completely sealed systems. Loading and unloading of tankers with sulphur trioxide for use as an intermediate is performed in the open air. Workers wear protective clothing (face/eye protection, helmet, anti-acid gloves boots and protective overall). A safety shower is required nearby in case of accidental spillage. Gas displacement lines are also used if filling of road tankers takes place under cover. If respiratory protection is required then it is used. For each subsequent industrial ES the same general routes of exposure as for production are relevant. In all cases the risk of worker exposure, as determined for each PROC, will be governed by the same exposure routes as production in many cases. For the environmental assessment the risk the emission levels (fractions) for each ES will be dictated by the relevant ERC however the routes of environmental exposure will remain the same with the majority of the emissions being

directed to the air (though they will be mostly removed by scrubbers) or to the liquid waste stream and to STP where conversion to sulphuric acid and neutralization will occur.

Operational conditions related to frequency, duration and amount of use

The intermediate use of sulphur trioxide is generally a continuous/batch production, with the process running for long periods without interruption, for up to 360 days per year. Operators work a standard shift and normal working week, with activity continuing at weekends.

Duration, frequency and amounts

Information type	Data field	Explanation
Use amount per worker [workplace] per day	No data	Worker exposure considered to be negligible due to the specialised systems and closed nature of the production process.
Duration per day at workplace [for one worker]	8hr/d	Standard number of hours in one work day
Frequency at workplace [for one worker]	220 d/y	Standard number of work days / year
Other determinants related to duration, frequency and amount of use	Intermittent contact is expected	These tasks rarely take a full 8hr / day so worst case is assumed.
Annual amount used per site	10,000 t/y	Worst case for single site
Emission days per site	360 d/y	Estimate number of emission days, based on continuous production

Operational conditions and risk management measures related to product characteristics

Product Characteristic

Information type	Data field	Explanation
Type of product the information relates to	Substance as such or substance in oleum	The product is in liquid form in a sealed tank container in both cases.
Physical state of product	Liquid	
Concentration of substance in product	> 98 %	

Operational conditions related to available dilution capacity and characteristics of exposed humans

Respiration volume and skin contact under conditions of worker uses

Information type	Data field	Explanation

Respiration volume under conditions of use	10m^3/d	Default value for a worker breathing for a 8hrs work day in RIP 3.2
Skin contact area with the substance under conditions of use	480cm^2 (ECETOC default)	Please note that due to the corrosive nature of sulphuric acid dermal exposure is not considered relevant for risk characterisation as it must be prevented in all cases.

Conditions leading to dilution of initial release related to human health

Information type	Data field	Explanation
Room size and ventilation rate	N/A	Not relevant as workers involved in production work in a control room, with no direct contact to the installations housing the material

Conditions leading to dilution of initial release related to environment

Information type	Data field	Explanation
Discharge volume of sewage treatment plant	2000 m^3/d	EUSES default value for standard local STP
Available river water volume to receive the emissions from a site	20,000 m^3/d	Standard ERC flow rate leading to a 10 fold dilution in receiving waters.

Risk management measures

Waste gasses are minimised and can be filtered and scrubbed if required typically this removes >99% of sulphur oxides. This removal has not been taken into account in the assessment below and so should be considered to be worst case.

Workers involved in processing, handing, sampling and transfer of materials are trained in the procedures and protective equipment is intended to cope with the worst case scenario, in order to minimise exposure and risks. This may include chemical resistant clothing, goggles and respiratory equipment where required. Due to the nature of the materials the level of control and system closure is extremely high and so in reality exposure is highly unlikely. Primary emission sources are not located in the breathing zone of the worker as workers are in a separate control room. The handling of sulphur trioxide is such that contact between product and adjacent air is reduced and controlled loading is used reducing the amount of aerosol formation. Vapour recovery systems and local exhaust ventilation such as enclosing hoods are used. Emission sources are completely segregated from the work environment by isolating the source in a fully enclosed and separate room and there is complete personal enclosure with ventilation. The processes are fully enclosed (air tight) and the integrity of the enclosure is monitored. The facilities are housed outdoors, not close to buildings and workers are generally located > 4 metres from far field source.

Environmental emissions are limited by designated waste treatment process designed to limit environmental exposure to all relevant compartments. Waste gas emissions are

scrubbed and may also then be diverted to the wastewater stream. This significantly lessens the possible emission by atmospheric deposition to soil or surface waters. Liquid wastes would generally contain sulphuric acid that has formed when sulphur trioxide contacts water and these converted wastes are treated (neutralisation to neutral pH) prior to emission to remove any sulphuric acid in the waste water and sludge from the waste water treatment plant is sent for incineration or landfill and is not used for agricultural spreading. This precludes any contamination of soil by sludge spreading. Waste water treatment is usually carried out by neutralisation followed by flocculation or decantation.

Risk management measures for industrial site

Information type	Data field	Explanation
Containment and local exhaust ventilation		
Containment plus good work practice required	Effectiveness: Unknown	Use of sulphur trioxide involves special equipment and high integrity contained systems with little or no potential for exposure. Facilities involved in the production and uses of sulphur trioxide are completely segregated from the work environment by isolating the source in a fully enclosed and separate room and there is complete personal enclosure with ventilation. The processes are fully enclosed (air tight) and the integrity of the enclosure is monitored. The facilities are housed outdoors, not close to buildings and workers are normally located > 4 metres from far field source.
Local exhaust ventilation is required	Effectiveness : Unknown	Vapour recovery systems and local exhaust ventilation such as enclosing hoods are used.
Personal protective equipment (PPE)		
Type of PPE (gloves, respirator, face-shield etc)	Effectiveness: Unknown	Workers involved in sampling and transfer of materials to road tankers are trained in the procedures and protective equipment is intended to cope with the worst case scenario, in order to minimise exposure and risks.
Other risk management measures related to workers		
Primary emission sources are not located in the breathing zone of the worker as workers are in a separate control room. The handling of sulphur trioxide is such that contact between product and adjacent air is reduced and submerged loading is used reducing the amount of aerosol formation.		
Risk management measures related to environmental emissions from industrial sites		
Onsite pre-treatment of waste water	Chemical pre-treatment or onsite STP.	Waste waters are generally treated on site by chemical neutralisation methods before release to the municipal STP or to the environment.
Resulting fraction of initially applied amount in waste water released from site to the external sewage system	Varies depending on system.	The neutralisation process is extremely efficient and pH monitors are in place to ensure that complete neutralisation and removal have taken place. Complete conversion of sulphur trioxide to sulphuric acid in the waste stream is expected.
Air emission abatement	Effectiveness: Adequate measures in place	Exhaust gases from the production treated by scrubbers.

Information type	Data field	Explanation
Onsite waste treatment	Effectiveness: complete	The waste water neutralisation process is extremely efficient with almost total neutralisation achieved. pH alarms are in place to ensure that successful neutralisation has taken place.
Effluent (of the waste water treatment plant) discharge rate	2000 m^3/d	Default: 2.000 m^3/d
Recovery of sludge for agriculture or horticulture	No	All sludge is collected and incinerated or sent to landfill.
Resulting fraction of initially applied amount in waste water released from site	Complete removal	In the second tier removal of formed sulphuric acid by neutralization has been considered.

Exposure estimation

Workers exposure

The assessment of worker exposure to sulphur trioxide used as an intermediate in the manufacture of sulphuric acid, organic and inorganic chemicals (ES 2) was carried for processes relevant to this use scenario as identified by PROC codes. Initially, a screening-level (Tier 1) assessment was carried out using the ECETOC Targeted Risk Assessment (TRA) model. A higher tier (Tier 2) refinement of the Tier 1 assessment was carried out using the Advanced REACH Tool (ART).

Acute/short -term and long-term exposure

Parameters used in the ECETOC TRA model to conduct a Tier 1 assessment of inhalation exposure concentrations

	Parameter	Explanation/source of data
Molecular weight	80.06 g/mol	
Vapour Pressure	9730 Pa	
Water solubility	10000 mg/L	Representative value used in modelling as sulphur trioxide rapidly hydrolyses in water to form sulphuric acid which is highly miscible.
Is the substance a solid?	No – liquid	
Dustiness during process	n/a	Only in the case of solid
Duration of activity	>4 hours (default)	
Use of ventilation	Indoors with LEV	
Use of respiratory protection	Yes, 95% efficiency	

Exposure concentrations to workers

Description of activity	PROC	Physical state of material	Estimated Exposure Concentrations*	
			value	unit
Production (High integrity closed system, sampling via closed loop)	1	Liquid	1.67×10^{-03}	mg/m^3
Production and sampling (Occasional exposure system)	2	Liquid	1.67×10^{-01}	mg/m^3
Production, transfer and sampling	3	Liquid	4.17×10^{-01}	mg/m^3
Production, transfer and sampling (Exposure likely)	4	Liquid	3.34×10^{-01}	mg/m^3
Loading/transfer	8b	Liquid	2.50×10^{-01}	mg/m^3
Loading/transfer (Small containers)	9	Liquid	8.34×10^{-01}	mg/m^3

Parameters and assumptions used in the ART model to conduct a Tier 2 assessment of inhalation exposure concentrations

	PROC	Parameters/ assumptions
Exposure duration	PROC 1,2,8b,9	480 min
	PROC 3,4	120 min
Product type	All	Liquid
Process temperature	PROC 1,2,3,4	Hot processes (50-150°C)
	PROC 8b, 9	Room temperature (15-25°C)
Vapour pressure	All	9730 pa
Liquid weight fraction	All	Pure liquid (100%)
Primary emission source proximity	All	Primary emission source is not located in the breathing zone of the worker - the assessment for this activity involves a primary far-field emission source only (workers are in a control room)
Activity class	All	Transfer of liquid products
Containment	PROC 1,2,3,9	Handling reduces contact between product and adjacent air, submerged loading
	PROC 4	Open process, submerged loading
	PROC 8b	n/a due to bottom loading
Localised controls	PROC 1,3,8b,9	Vapour recovery systems; LEV
	PROC 2,4	Vapour recovery
Segregation	PROC 1,2,9	Complete segregation of workers in separate control room

	PROC 3,4,8b	Partial segregation of workers
Fugative emission source	PROC 1,8b,9	Process fully enclosed – not breached for sampling
	PROC 2,3,4	Not fully enclosed – effective housekeeping practices in place.
Dispersion	PROC 1,2	Outdoors not close to buildings, worker located >4 meters from far field source
	PROC 3,4,8b	Outdoors close to buildings, worker located >4 meters from far field source
	PROC 9	Indoors, any sized room, only good natural ventilation

Tier 2 acute/short-term and long-term inhalation exposure concentrations derived using the ART model

Description of activity	**PROC**	**Physical state of material**	**Estimated Short-term Exposure Concentrations (mg/m3)**		**Estimated Long-term Exposure Concentration (mg/m3)**	
			50th percentile value	**90th percentile value**	**50th percentile value**	**90th percentile value**
Production (High integrity closed system, sampling via closed loop)	1	Liquid	2.2×10^{-04}	1.5×10^{-03}	5.4×10^{-04}	1.3×10^{-03}
Production and sampling (Occasional exposure system)	2	Liquid	2.2×10^{-03}	1.5×10^{-02}	5.4×10^{-03}	1.3×10^{-02}
Production, transfer and sampling	3	Liquid	2.0×10^{-04}	1.3×10^{-03}	4.9×10^{-04}	1.1×10^{-03}
Production, transfer and sampling (Exposure likely)	4	Liquid	6.7×10^{-03}	4.4×10^{-02}	1.6×10^{-02}	3.8×10^{-02}
Loading/transfer	8b	Liquid	2.2×10^{-03}	1.5×10^{-02}	5.4×10^{-03}	1.3×10^{-02}
Loading/transfer (Small containers)	9	Liquid	1.1×10^{-02}	3.3×10^{-02}	1.3×10^{-02}	2.9×10^{-02}

Consumer exposure

Consumers are not directly exposed to sulphur trioxide during the processes associated with ES1 as this exposure scenario involves only closed industrial processes.

Indirect exposure of humans via the environment (oral)

Environmental exposure

Intermediate use of sulphur trioxide is generally a continuous process with constant production and use throughout the year. Facilities may generally utilise sulphur trioxide at

up to 360 days per year.
First tier conservative environmental exposure estimations were carried out using EUSES 2.1 and using the specified defaults. ERC 6A was used to determine the environmental emissions for intermediate use in the first tier with more realistic refined inputs chosen for second tier assessment. 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 and partitioning including degradation and sorption parameters. As the tier 1 assessment was not considered to give a reasonable or satisfactory assessment only the results of the second tier assessment has been shown below.

Environmental releases

EUSES inputs for intermediate use of sulphuric acid

Input parameter:	Value:	Unit:	ERC default (if applicable)
Molecular Weight	80.06	g/mol	
Vapour Pressure (at 25 °C)	9730	hPa	
Water Solubility	1000	mg/L	
Octanol/water partition coefficient	-1 (estimated)	logKow	
Koc	1 (estimated)		
Biodegradability	Not biodegradable (inorganic oxides cannot be considered biodegradable)		
Life Cycle Step	Industrial use		
Environmental Release Class	ERC 6A		
Fraction of Tonnage for Region (1st Tier)			1
STP			Yes
Emission events per year	360 (manufacturer information)	Days	300 (based on tonnage and use band)
Default Release to Air	5	%	5
Default Release to water	2	%	2
Dilution factor applied for PEC derivation			10 (20,000 m^3/d)

Input parameter:	Value:	Unit:	ERC default (if applicable)
Local tonnage assessed	10,000	tonnes/annum	Worst case single site use rate

For the tier 2 assessment of environmental releases the effects of several RMMs have been investigated alongside the worst case measured values obtained from consortium members to cover the use of sulphur trioxide as an intermediate.

RMMs and measured values for tier 2 assessment.

Description of RMM	Details	Effect taken into account in EUSES	Comments
No loss to waste water	0 mg/L	Lowering of concentration in STP effluent to 0 mg/L due to the conversion of sulphur trioxide to sulphuric acid and the very efficient neutralization process to remove sulphuric acid in the waste stream	Total neutralization to around pH 7.
Emission and production days	360 emission days per year	Increase emission days by 20%.	Continuous production
Sludge removal	Sludge removed to landfill or incinerated.	Concentration in soil due to sludge spreading set to 0.	No contamination of grassland or agricultural soil.

Predicted Releases to the Environment Tier 2

ERC	Compartments	Predicted releases	Measured release	Explanation / source of measured data
6A	Aquatic freshwater (after STP)	833kg/d	-	Predicted values are those calculated by EUSES using the tonnage data and defaults for ERC6A.
	Release to air	2,080 kg/d	-	Predicted values are those calculated by EUSES using the tonnage data and defaults for ERC6A
	Soil (direct only) Agricultural soil	0 kg/d	-	No directly loss to soil is expected for this ERC and no sludge spreading.

ES 3: Use of oleum as a nitration agent

Sector of Use:

SU3: Industrial uses: Uses of substances as such or in preparation at industrial sites
SU8: Manufacture of bulk, large scale chemicals (including petroleum products)
SU9: Manufacture of fine chemicals

Produce Category:

PC20: Products such as ph-regulators, flocculants, precipitants, neutralization agents
PC21: Laboratory chemicals

Process Categories:

PROC01: Use in closed process, no likelihood of exposure
PROC02: Use in closed, continuous process with occasional controlled exposure
PROC03: Use in closed batch process (synthesis or formulation)
PROC04: Use in batch and other process (synthesis) where opportunity for exposure arises
PROC08b: Transfer of substance or preparation (charging/discharging) from/to vessels/large containers at dedicated facilities
PROC09: Transfer of substance or preparation into small containers (dedicated filling line, including weighing)
PROC15: Use as laboratory reagent

Environmental Release Category:

ERC06b: Industrial use of reactive processing aids

Description of activities and processes covered in the exposure scenario

For ES3 the processes utilising sulphur trioxide as a component in nitrating agents are in principle similar to the processes for previous exposure scenarios with regards to the degree of control and system closure. The processes associated with this exposure scenario would generally take place in large commercial industrial laboratories and the large size of the typical facility involved means that all processes are carried out in a controlled environment by highly trained workers with high levels of exposure limiting measures and containment in place. Furthermore waste capture strategies including the use of flow hoods with gaseous removal and dedicated effluent capture treatment facilities are generally employed.

It is expected that should such operations be carried out sufficient emission and exposure control measures are put in place to protect those carrying out the laboratory work and

the environment.

Operational conditions related to frequency, duration and amount of use

The industrial scale laboratory use of sulphur trioxide as a component of nitrating agents may run as a continuous process with up to 330 days utilisation per year. Laboratory workers can be considered work a standard shift and normal working week thought actual exposure time to sulphur trioxide would be significantly less than the total time spent in the laboratory.

Duration, frequency and amounts

Information type	Data field	Explanation
Use amount per worker [workplace] per day	No data	Worker exposure considered to be negligible due to the specialised systems and closed nature of the production process.
Duration per day at workplace [for one worker]	8h/d	Standard number of hours in one work day
Frequency at workplace [for one worker]	220 d/y	Standard number of work days / year
Other determinants related to duration, frequency and amount of use	Intermittent contact is expected thought there are measures in place to ensure that in reality no exposure occurs	These tasks rarely take a full 8h / day so worst case is assumed.
Annual amount used per site	5,000 t/y	Worst case estimation based on a very large industrial laboratory
Emission days per site	330 d/y	Estimate number of emission days, based on continuous production

Operational conditions and risk management measures related to product characteristics

Product Characteristic

Information type	Data field	Explanation
Type of product the information relates to	Substance as such	The product is in liquid form in a sealed

Information type	Data field	Explanation
		tank container.
Physical state of product	Liquid	
Concentration of substance in product	Generally around 20-25%	Concentration in the nitration mixture is generally lower however formulations of 20-25% of sulphur trioxide are commonly supplied.

Remarks or additional information:
Use of sulphur trioxide as a component in nitrating mixtures involves high integrity controlled systems with little or no potential for exposure. Pipelines and vessels are sealed. Laboratory workers are trained in the procedures and protective equipment is intended to cope with the worst case scenario, in order to minimise exposure and risks.

Operational conditions related to available dilution capacity and characteristics of exposed humans

Respiration volume and skin contact under conditions of worker uses

Information type	Data field	Explanation
Respiration volume under conditions of use	$10m^3/d$	Default value for a worker breathing for a 8h work day in RIP 3.2
Skin contact area with the substance under conditions of use	$480cm^2$ (ECETOC default)	Please note that due to the corrosive nature of sulphuric acid dermal exposure is not considered relevant for risk characterisation as it must be prevented in all cases.

Conditions leading to dilution of initial release related to human health

Information type	Data field	Explanation
Room size and ventilation rate	Large industrial laboratory with sufficient controlled segregation and ventilation	Exact size and ventilation will vary

Conditions leading to dilution of initial release related to environment

Information type	Data field	Explanation
Discharge volume of sewage treatment plant	2000 m^3/d	EUSES default value for standard local STP
Available river water volume to receive the emissions from a site	20,000 m^3/d	Standard ERC flow rate leading to a 10 fold dilution in receiving waters.

As described in previous exposure scenarios the handling of sulphur trioxide involves special equipment and highly specialised contained systems with little or no potential for exposure.

Risk management measures

Workers involved in the industrial laboratory use of sulphur trioxide as a nitrating agent component are generally highly trained with regards to the handling of the substance, proper segregation of the substance and the use of appropriate RPE and emission/exposure control measures. Protective equipment is intended to cope with the worst case scenario, in order to minimise exposure and risks. This may include chemical resistant clothing, goggles, vapour removal, substance segregation, system closure and respiratory equipment where required.

Environmental emissions are limited by designated waste treatment process designed to limit environmental exposure to all relevant compartments. General sulphide waste gas emissions are scrubbed and may also then be diverted to the wastewater stream. This significantly lessens the possible emission by atmospheric deposition to soil or surface waters. Liquid wastes are treated (neutralisation of the formed sulphuric acid to neutral pH) prior to emission to remove any sulphuric acid in the waste water and sludge from the waste water treatment plant is sent for incineration or landfill and is not used for agricultural spreading. This precludes any contamination of soil by sludge spreading. Waste water treatment is usually carried out by neutralisation followed by flocculation or decantation.

Risk management measures for industrial site

Information type	Data field	Explanation
Containment and local exhaust ventilation		
Containment plus good work practice required	Effectiveness: Unknown	Handling of sulphur trioxide involves special equipment and high integrity contained systems with little or no potential for exposure. Facilities involved in the uses of sulphur trioxide are usually strictly contained. Any gas displaced from containers is conducted via pipeline to be processed i.e. removed and scrubbed and /or filtered to limit worker exposure.

Information type	Data field	Explanation
Local exhaust ventilation	Effectiveness : Unknown	Local gas removal and filtering should be on site in laboratories and facilities that use sulphuric acid as a nitrating agent component. Flow hoods and glove boxes should be used when required.
Personal protective equipment (PPE)		
Type of PPE (gloves, respirator, face-shield etc)	Effectiveness: Unknown	Workers involved in sampling and transfer of materials to road tankers are trained in the procedures and protective equipment is intended to cope with the worst case scenario, in order to minimise exposure and risks.
Other risk management measures related to workers		
Systems handling sulphur trioxide should be properly contained and workers should be segregated from any possible emissions		
Risk management measures related to environmental emissions from industrial sites		
Onsite pre-treatment of waste water	Chemical pre-treatment or onsite STP.	Waste waters are generally treated on site by chemical neutralisation methods before release to the municipal STP or to the environment.
Resulting fraction of initially applied amount in waste water released from site to the external sewage system	Varies depending on system.	The neutralisation process is extremely efficient and pH monitors are in place to ensure that complete neutralisation and removal have taken place. Complete conversion of sulphur trioxide to sulphuric acid in the waste stream is expected.
Air emission abatement	Effectiveness: Adequate measures in place	Exhaust gases from the production treated by scrubbers.
Onsite waste treatment	Effectiveness: complete	The waste water neutralisation process is extremely efficient with almost total neutralisation achieved. pH alarms are in place to ensure that successful neutralisation has taken place.
Effluent (of the waste water treatment plant) discharge rate	2000 m^3/d	Default: 2.000 m^3/d
Recovery of sludge for agriculture or horticulture	No	All sludge is collected and incinerated or sent to landfill.
Resulting fraction of initially applied amount in waste water released from site	Complete removal	In the second tier removal of formed sulphuric acid by neutralization has been considered.

Exposure estimation

Workers exposure

The assessment of worker exposure to sulphur trioxide used during the nitration of chemicals (ES 3) was carried for processes relevant to this use scenario as identified by PROC codes. Initially, a screening-level (Tier 1) assessment was carried out using the ECETOC Targeted Risk Assessment (TRA) model. A higher tier (Tier 2) refinement of the Tier 1 assessment was carried out using the Advanced REACH Tool (ART).

Acute/short -term and long-term exposure

Parameters used in the ECETOC TRA model to conduct a Tier 1 assessment of inhalation exposure concentrations

	Parameter	Explanation/source of data
Molecular weight	80.06 g/mol	
Vapour Pressure	9730 Pa	
Water solubility	10000 mg/L	Representative value used in modelling as sulphur trioxide rapidly hydrolyses in water to form sulphuric acid which is highly miscible.
Is the substance a solid?	No – liquid	
Dustiness during process	n/a	Only in the case of solid
Duration of activity	>4 hours (default)	
Use of ventilation	Indoors with LEV	
Use of respiratory protection	Yes, 95% efficiency	

Tier 1 inhalation exposure concentrations derived using the ECETOC TRA model

Description of activity	PROC	Physical state of material	Estimated Exposure Concentrations	
			value	unit
Production (High integrity closed system, sampling via closed loop)	1	Liquid	1.67×10^{-03}	mg/m^3
Production and sampling (Occasional exposure system)	2	Liquid	1.67×10^{-01}	mg/m^3
Production, transfer and sampling: Use of sulphuric acid in a closed batch process	3	Liquid	4.17×10^{-01}	mg/m^3
Production, transfer and sampling : Use of sulphuric acid in batch processes (exposure likely)	4	Liquid	3.34×10^{-01}	mg/m^3
Loading/transfer: Loading and unloading a tanker (dedicated site)	8b	Liquid	2.50×10^{-01}	mg/m^3
Loading/transfer (filling small containers with sulphuric acid)	9	Liquid	8.34×10^{-01}	mg/m^3
Laboratory chemicals	15	Liquids	1.67×10^{-01}	mg/m^3

Parameters and assumptions used in the ART model to conduct a Tier 2 assessment of inhalation exposure concentrations

	PROC	Parameters/ assumptions
Exposure duration	PROC 1,2,8b,9	480 min
	PROC 3,4,15	120 min
Product type	All	Liquid
Process temperature	PROC 1,2,3,4	Hot processes (50-150°C)
	PROC 8b, 9,15	Room temperature (15-25°C)
Vapour pressure	All	9730 pa
Liquid weight fraction	All	Substantial component (10-50%)
Primary emission source proximity	PROC 1,2,3,4,8b,9	Primary emission source is not located in the breathing zone of the worker - the assessment for this activity involves a primary far-field emission source only (workers are in a control room)
	PROC 15	Primary emission source is located in the breathing zone of the worker (i.e. Within a metre)
Activity class	All	Transfer of liquid products
Containment	PROC 1,2,3,9	Handling reduces contact between product and adjacent air, submerged loading
	PROC 4	Open process, submerged loading
	PROC 8b	n/a due to bottom loading
	PROC 15	Open process, splash loading
Localised controls	PROC 1,3,8b,9	Vapour recovery systems; LEV
	PROC 2,4	Vapour recovery
	PROC 15	LEV; glove boxes
Segregation	PROC 1,2,9	Complete segregation of workers in separate control room
	PROC 3,4,8b	Partial segregation of workers
	PROC 15	n/a
Fugative emission source	PROC 1,8b,9	Process fully enclosed – not breached for sampling
	PROC 2,3,4,15	Not fully enclosed – effective housekeeping practices in place.
Dispersion	PROC 1,2	Outdoors not close to buildings, worker located >4

		meters from far field source
	PROC 3,4,8b	Outdoors close to buildings, worker located >4 meters from far field source
	PROC 9,15	Indoors, any sized room, only good natural ventilation

Tier 2 acute/short-term and long-term inhalation exposure concentrations derived using the ART model

Description of activity	PROC	Physical state of material	Estimated Short-term Exposure Concentrations (mg/m3)		Estimated Long-term Exposure Concentration (mg/m3)	
			50th percentile Value	90th percentile value	50th percentile value	90th percentile value
Production (High integrity closed system, sampling via closed loop)	1	Liquid	6.8×10^{-05}	4.5×10^{-04}	1.6×10^{-04}	3.8×10^{-04}
Production and sampling (Occasional exposure system)	2	Liquid	6.7×10^{-04}	4.5×10^{-03}	1.6×10^{-03}	3.8×10^{-03}
Production, transfer and sampling: Use of sulphuric acid in a closed batch process	3	Liquid	6.1×10^{-05}	4.0×10^{-04}	1.5×10^{-04}	3.5×10^{-04}
Production, transfer and sampling : Use of sulphuric acid in batch processes (exposure likely)	4	Liquid	2.0×10^{-03}	1.3×10^{-02}	4.9×10^{-03}	1.1×10^{-02}
Loading/transfer: Loading and unloading a tanker (dedicated site)	8b	Liquid	6.7×10^{-04}	4.5×10^{-03}	1.6×10^{-03}	3.8×10^{-03}
Loading/transfer (filling small containers with sulphuric acid)	9	Liquid	3.2×10^{-03}	9.9×10^{-03}	3.8×10^{-03}	8.7×10^{-03}
Laboratory chemicals	15	Liquids	6.3×10^{-04}	2.0×10^{-03}	7.6×10^{-04}	1.7×10^{-03}

Consumer exposure

Consumers are not directly exposed to sulphur trioxide during the activities covered under this exposure scenario as they are purely industrial and there is no direct release to consumers.

Indirect exposure of humans via the environment (oral)

Indirect exposure of humans via the environment is expected to be negligible. Sulphur trioxide converts to sulphuric acid upon contact with environmental moisture. This sulphuric acid is fully miscible in water and, as such, will not persist in any environmental compartment where indirect exposure of humans could occur. Furthermore none of the processes associated with sulphur trioxide production involve any targeted environmental emissions or application and the primary receiving compartment is the on-site STP where rigorous neutralisations processes and employed. Removal in the STP is expected to be efficient and so secondary exposure of the other receiving compartments is expected to be minimal. Similarly contamination of food crops or animals used as human food sources is not envisaged.

EUSES inputs for environmental assessment

Input parameter:	Value:	Unit:	ERC default (if applicable)
Molecular Weight	80.06	g/mol	
Vapour Pressure (at 25 °C)	9730	hPa	
Water Solubility	1000	mg/L	
Octanol/water partition coefficient	-1 (estimated)	logKow	
Koc	1 (estimated)		
Biodegradability	Not biodegradable (inorganic oxides cannot be considered biodegradable)		
Life Cycle Step	Industrial use		
Environmental Release Class	ERC 6B		
Fraction of Tonnage for Region (1st Tier)			1
STP			Yes
Emission events per year	360 (manufacturer information)	Days	300 (bases on tonnage band and use)
Default Release to Air for ERC 6B	0.10	%	0.10
Default Release to Water for ERC 6B	5	%	5
Dilution factor applied for PEC derivation			10 (20,000 m^3/d)
Tonnage assessed	5,000	tonnes/annum	Local site worst case tonnage

For the tier 2 assessment of environmental releases the effects of several RMMs have been investigated alongside the worst case measured values obtained from consortium

members to cover the use of sulphur trioxide in the nitration process.

RMMs and measured values for tier 2 assessment.

Description of RMM	Details	Effect taken into account in EUSES	Comments
No loss to waste water	0 mg/L	Lowering of concentration in STP effluent to 0 mg/L due to the conversion of sulphur trioxide to sulphuric acid and the very efficient neutralization process to remove sulphuric acid in the waste stream	Total neutralization to around pH 7.
Emission and production days	360 emission days per year	Increase emission days by 20%.	Continuous production
Sludge removal	Sludge removed to landfill or incinerated.	Concentration in soil due to sludge spreading set to 0.	No contamination of grassland or agricultural soil.

Predicted Releases to the Environment Tier 2

ERC	Compartments	Predicted releases	Measured release	Explanation / source of measured data
6B	Aquatic freshwater (after STP)	0 kg/d	-	Based on effective neutralization and pre-treatment
	Release to air	13.9kg/d	-	Predicted values are those calculated by EUSES using the tonnage data and defaults for ERC6B. No refinement needed.
	Soil (direct only) Agricultural soil	0 kg/d	-	No directly loss to soil is expected for this ERC and no sludge spreading.

ES 4: Formulation of oleum

Sector of Use:

SU10: Formulation [mixing] of preparations and/or re-packaging (excluding alloys)

Process Categories:

PROC01: Use in closed process, no likelihood of exposure
PROC08b: Transfer of substance or preparation (charging/discharging) from/to vessels/large containers at dedicated facilities
PROC09: Transfer of substance or preparation into small containers (dedicated filling line, including weighing)

Environmental Release Category:

ERC02: Formulation of preparations

Description of activities and processes covered in the exposure scenario

For ES4 the processes utilising sulphur trioxide in the manufacture of oleum are largely similar to those discussed for ES1 with regards to the degree of control and system closure. Generally the formulation process would be continuous with use levels ranging between 100 and 200 tonnes per day in a large facility. The large size of the typical facility involved means that all vessels and reactors are housed out-doors, managed by a small number of operators working in a separate enclosed control room.

Loading and unloading of tankers with oleum is usually performed in the open air. Workers wear protective clothing (face/eye protection, helmet, anti-acid gloves boots and protective overall). A safety shower is required nearby in case of accidental spillage. Gas displacement lines are also used if filling of road tankers takes place under cover. System containment and segregation is in place to ensure that exposure does not occur.

Operational conditions related to frequency, duration and amount of use

The industrial scale formulation of oleum is generally a continuous production process, running for long periods without interruption, for up to 360 days per year. Operators work a standard shift and normal working week, with production continuing at weekends.

Table 1:Duration, frequency and amounts

Information type	Data field	Explanation
Use amount per worker [workplace] per day	No data	Worker exposure considered to be negligible due to the specialised systems and closed nature of the oleum formulation process.

Information type	Data field	Explanation
Duration per day at workplace [for one worker]	8hr/d	Standard number of hours in one work day
Frequency at workplace [for one worker]	220 d/year	Standard number of work days / year
Other determinants related to duration, frequency and amount of use	Intermittent contact is expected	These tasks rarely take a full 8hr / day so worst case is assumed.
Annual amount used per site	75,000 t/y	Worst case for single production site
Emission days per site	Up to 360	Estimate number of emission days, based on continuous production

Operational conditions and risk management measures related to product characteristics

Product Characteristics

Information type	Data field	Explanation
Type of product the information relates to	Substance in oleum	The product is in liquid form in a sealed tank container.
Physical state of product	Liquid	
Concentration of substance in product	Produced SO_3 > 98 % in oleum 20 -25%	SO_3 is dissolved in sulphuric acid to form oleum

Remarks or additional information:

Use of sulphur trioxide involves high temperatures (during the incineration of molten sulphur) and high integrity contained systems with little or no potential for exposure. Pipelines and vessels are sealed. Workers involved in production work in a separate control room, with no direct contact to the installations housing the material. Workers involved in sampling and transfer of materials to road tankers are trained in the procedures and protective equipment is intended to cope with the worst case scenario, in order to minimise exposure and risks.

Operational conditions related to available dilution capacity and characteristics of exposed humans

Respiration volume and skin contact under conditions of worker uses

Information type	Data field	Explanation
Respiration volume under conditions of use	$10m^3/d$	Default value for a worker breathing for a 8h work day in RIP 3.2
Skin contact area with the substance under conditions of use	$480cm^2$ (ECETOC default)	Please note that due to the corrosive nature of sulphuric acid dermal exposure is not considered relevant for risk characterisation as it must be prevented in all cases.

Conditions leading to dilution of initial release related to human health

Information type	Data field	Explanation
Room size and ventilation rate	NA	Not relevant as workers involved in production work in a control room, with no direct contact to the installations housing the material

Conditions leading to dilution of initial release related to environment

Information type	Data field	Explanation
Discharge volume of sewage treatment plant	2000 m^3/d	EUSES default value for standard local STP
Available river water volume to receive the emissions from a site	20,000 m^3/d	Standard ERC flow rate leading to a 10 fold dilution in receiving waters.

Formulation and handling of sulphur trioxide involves specialized processes, special equipment and high integrity contained systems with little or no potential for exposure. Facilities involved in the production and uses of sulphur trioxide are usually housed outdoors. Any gas displaced from containers (which is normally not the case due to the high level of system closure) is conducted via pipeline to be processed i.e. removed and scrubbed and /or filtered. Note that there is direct consumer use of sulphuric acid.

Risk management measures

Workers involved in formulation, handing, sampling and transfer of materials are trained in the procedures and protective equipment is intended to cope with the worst case scenario, in order to minimise exposure and risks. This may include chemical resistant clothing, goggles and respiratory equipment where required. There is a high degree of system closure. Primary emission sources are not located in the breathing zone of the worker as workers are in a separate control room. The handling of sulphur trioxide is such that contact between product and adjacent air is reduced and controlled submerged loading is used reducing the amount of aerosol formation. Vapour recovery systems and local exhaust ventilation such as enclosing hoods are used. Emission sources are completely segregated from the work environment by isolating the source in a fully enclosed and separate room and there is complete personal enclosure with ventilation. The processes are fully enclosed (air tight) and the integrity of the enclosure is monitored. The facilities are generally housed outdoors, not close to buildings and workers normally are located > 4 metres from far field source.

Environmental emissions are limited by designated waste treatment process designed to limit environmental exposure to all relevant compartments. Waste gas emissions are scrubbed and may also then be diverted to the wastewater stream. This significantly lessens the possible emission by air deposition to soil or surface waters. Liquid wastes are treated (neutralisation to neutral pH) prior to emission to remove any sulphuric acid in the waste water and sludge from the waste water treatment plant is sent for incineration or landfill and is not used for agricultural spreading. This precludes any contamination of soil by sludge spreading. Waste water treatment is usually carried out by neutralisation followed by flocculation or decantation.

Risk management measures for industrial site

Information type	Data field	Explanation
Containment and local exhaust ventilation		
Containment plus good work practice required	Effectiveness: Unknown	Production and handling of oleum using sulphur trioxide involves special equipment and high integrity contained systems with little or no potential for exposure. Facilities involved in the production and uses of sulphur trioxide are completely segregated from the work environment by isolating the source in a fully enclosed and separate room and there is complete personal enclosure with ventilation. The processes are fully enclosed (air tight) and the integrity of the enclosure is monitored. The facilities are housed outdoors, not close to buildings and workers are usually located > 4 metres from far field source.
Local exhaust ventilation is not required	Effectiveness : Unknown	Vapour recovery systems and local exhaust ventilation such as enclosing hoods are used.
Personal protective equipment (PPE)		
Type of PPE (gloves, respirator, face-shield etc)	Effectiveness: Unknown	Workers involved in sampling and transfer of materials to road tankers are trained in the procedures and protective equipment is intended to cope with the worst case scenario, in order to minimise exposure and risks.
Other risk management measures related to workers		
Primary emission sources are not located in the breathing zone of the worker as workers are in a separate control room. The handling of sulphur trioxide is such that contact between product and adjacent air is reduced and submerged loading is used reducing the amount of aerosol formation.		

Information type	Data field	Explanation
Risk management measures related to environmental emissions from industrial sites		
Onsite pre-treatment of waste water	Chemical pre-treatment or onsite STP.	Waste waters are generally treated on site by chemical neutralisation methods before release to the municipal STP or to the environment.
Resulting fraction of initially applied amount in waste water released from site to the external sewage system	Varies depending on system.	The neutralisation process is extremely efficient and pH monitors are in place to ensure that complete neutralisation and removal have taken place. Complete conversion of sulphur trioxide to sulphuric acid in the waste stream is expected.
Air emission abatement	Effectiveness: Adequate measures in place	Exhaust gases from the production treated by scrubbers.
Onsite waste treatment	Effectiveness: complete	The waste water neutralisation process is extremely efficient with almost total neutralisation achieved. pH alarms are in place to ensure that successful neutralisation has taken place.
Effluent (of the waste water treatment plant) discharge rate	2000 m^3/d	Default: 2.000 m^3/d
Recovery of sludge for agriculture or horticulture	No	All sludge is collected and incinerated or sent to landfill.
Resulting fraction of initially applied amount in waste water released from site	Complete removal	In the second tier removal of formed sulphuric acid by neutralization has been considered.

Exposure estimation

Workers exposure

The assessment of worker exposure to sulphur trioxide (and subsequent sulphuric acid mists in air) from production (ES4) was carried for processes relevant to this use scenario as identified by PROC codes. Initially, a screening-level (Tier 1) assessment was carried out using the ECETOC Targeted Risk Assessment (TRA) model. A higher tier (Tier 2) refinement of the Tier 1 assessment was carried out using the Advanced REACH Tool (ART).

Parameters used in the ECETOC TRA model to conduct a Tier 1 assessment of inhalation exposure concentrations

	Parameter	Explanation/source of data
Molecular weight	80.06 g/mol	
Vapour Pressure	9730 Pa	
Water solubility	10000 mg/L	Representative value used in modelling as sulphur trioxide

		rapidly hydrolyses in water to form sulphuric acid which is highly miscible.
Is the substance a solid?	No – liquid	
Dustiness during process	n/a	Only in the case of solid
Duration of activity	>4 hours (default)	
Use of ventilation	Indoors with LEV	
Use of respiratory protection	Yes, 95% efficiency	

Tier 1 inhalation exposure concentrations derived using the ECETOC TRA model

Description of activity	PROC	Physical state of material	Estimated Exposure Concentrations	
			value	unit
Production (High integrity closed system, sampling via closed loop)	1	Liquid	1.67 x10^{-03}	mg/m^3
Transfer of substances from/to vessels/large containers at dedicated facilities	8b	Liquid	2.50 x10^{-01}	mg/m^3
Transfer of substance into small containers (dedicated filling line - vapor/aerosol control)	9	Liquid	8.34 x10^{-01}	mg/m^3

Parameters and assumptions used in the ART model to conduct a Tier 2 assessment of inhalation exposure concentrations

	PROC	Parameters/ assumptions
Exposure duration	All	480 min
Product type	All	Liquid
Process temperature	PROC 1	Hot processes (50-150°C)
	PROC 8b, 9	Room temperature (15-25°C)
Vapour pressure	All	9730 pa
Liquid weight fraction	All	Substantial component (10-50%)
Primary emission source proximity	All	Primary emission source is not located in the breathing zone of the worker - the assessment for this activity involves a primary far-field emission source only (workers are in a control room)
Activity class	All	Transfer of liquid products

Containment	PROC 1,9	Handling reduces contact between product and adjacent air, submerged loading
	PROC 8b	n/a due to bottom loading
Localised controls	All	Vapour recovery systems; LEV
Segregation	PROC 1,9	Complete segregation of workers in separate control room
	PROC 8b	Partial segregation of workers
Fugative emission source	All	Process fully enclosed – not breached for sampling
Dispersion	PROC 1	Outdoors not close to buildings, worker located >4 meters from far field source
	PROC 8b	Outdoors close to buildings, worker located >4 meters from far field source
	PROC 9	Indoors, any sized room, only good natural ventilation

Tier 2 acute/short-term and long-term inhalation exposure concentrations derived using the ART model

Description of activity	PROC	Physical state of material	Estimated Short-term Exposure Concentrations (mg/m3)		Estimated Long-term Exposure Concentration (mg/m3)	
			50th percentile value	90th percentile value	50th percentile value	90th percentile value
Production (High integrity closed system, sampling via closed loop)	1	Liquid	6.8×10^{-05}	4.5×10^{-04}	1.6×10^{-04}	3.8×10^{-04}
Transfer of substances from/to vessels/large containers at dedicated facilities	8b	Liquid	6.7×10^{-04}	4.5×10^{-03}	1.6×10^{-03}	3.8×10^{-03}
Transfer of substance into small containers (dedicated filling line - vapour/aerosol control)	9	Liquid	3.2×10^{-03}	9.9×10^{-03}	3.8×10^{-03}	8.7×10^{-03}

Consumer exposure

Consumers are not directly exposed to sulphur trioxide during the processes associated with ES4 as this exposure scenario involves only closed industrial processes.

Indirect exposure of humans via the environment (oral)

Indirect exposure of humans via the environment is expected to be negligible. Sulphur trioxide converts to sulphuric acid upon contact with environmental moisture. This

EUSES inputs

Input parameter:	Value:	Unit:	ERC default (if applicable)
Molecular Weight	80.06	g/mol	
Vapour Pressure (at 25 °C)	9730	hPa	
Water Solubility	1000	mg/L	
Octanol/water partition coefficient	-1 (estimated)	logKow	
Koc	1 (estimated)		
Biodegradability	Not biodegradable (inorganic oxides cannot be considered biodegradable)		
Life Cycle Step	Formulation		
Environmental Release Class	ERC2		
Fraction of Tonnage for Region (1st Tier)			1
STP			Yes
Emission events per year	330 (manufacturer information)	Days	20
Default Release to Air for worst case ERC	2.5	%	2.5
Default Release to water	2	%	2
Dilution factor applied for PEC derivation			10 (20,000 m^3/d)
Tonnage assessed	75,000	tonnes/annum	Worst case site formulation value

For the tier 2 assessment of environmental releases the effects of several RMMs have been investigated.

RMMs and measured values for tier 2 assessment.

Description of RMM	Details	Effect taken into account in EUSES	Comments
No loss to waste water	0 mg/L	Lowering of concentration in STP effluent to 0 mg/L due to the conversion of sulphur trioxide to sulphuric acid and the very efficient neutralization process to remove sulphuric acid in the waste stream	Total neutralization to around pH 7.
Emission and production days	360 emission days per year	Increase emission days by 20%.	Continuous production
Sludge removal	Sludge removed to landfill or incinerated.	Concentration in soil due to sludge spreading set to 0.	No contamination of grassland or agricultural soil.

Predicted Releases to the Environment Tier 2

ERC	Compartments	Predicted releases	Measured release	Explanation / source of measured data
2	Aquatic freshwater (after STP)	0 kg/d	-	Based on efficient neutralization
	Release to air	5,210 kg/d	-	No refinement of the emission amounts is required
	Soil (direct only) Agricultural soil	0 kg/d	-	No directly loss to soil is expected for this ERC and no sludge spreading.