



Project No 327341, ACT 3 – Accelerating CCS Technologies

SCOPE

Sustainable OPERation of post-combustion
Capture plants (SCOPE)

PNECs and degradation data for amines and amine degradation products Deliverable D3.1

Deliverable no:	D3.3	
WP:	WP3	
Dissemination level:	Public	
Written by:	Odd Gunnar Brakstad, Bjørn Henrik Hansen, Maria Lathouri & Anna Korre	Date: 30.01.2023
Checked by:	Hanne Kvamsdal	Date: 03.02.2023
Issue date:	03.02.2023	



Document	Deliverable D3.1
Issue date	03 Feb 2023
Dissemination level	Public

Version	Author	Partner	Date	Status
v.1	Odd Gunnar Brakstad, Bjørn Henrik Hansen, Maria Lathouri & Anna Korre	SINTEF Ocean, Trondheim, Norway, Imperial College London, UK	16.12.2022	Draft
v.2	Odd Gunnar Brakstad, Bjørn Henrik Hansen, Maria Lathouri & Anna Korre	SINTEF Ocean, Trondheim, Norway, Imperial College London, UK	21.12.2022	Draft after internal QA (Lisbet Sørensen)
v.3	Odd Gunnar Brakstad, Bjørn Henrik Hansen, Maria Lathouri & Anna Korre	SINTEF Ocean, Trondheim, Norway, Imperial College London, UK	16.01.2023	Final
V4	Odd Gunnar Brakstad, Bjørn Henrik Hansen, Maria Lathouri & Anna Korre	SINTEF Ocean, Trondheim, Norway, Imperial College London, UK	30.01.2023	Final, small erratum

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Abbreviations

Abbreviation	Definition
AB	4-Amino-1-butanol
ACHP	1-amino-1-cyclohexylaminopropane
ACR	Acute to Chronic Ratios
AE-PZ	1-(2-Aminoethyl)piperazine
AEEA	N-(2-Hydroxyethyl)ethylenediamine
AEPD	2-Amino-2-ethyl-1,3-propanediol
AF	Assessment Factor
Ala	Alanine
AMOR	4-acetylmorpholine
AMP	2-Amino-2-methylpropanol
AMP-NO ₂	2-methyl- 2-(nitroamine)-1-propanol
AMPD	2-Amino-2-methyl-1,3-propanediol
AP	3-Aminopropanol
ASTM	American Society for Testing and Materials
BAT	Best Available Technique
BCF	Bioconcentration Factor
BEF	Best Environmental Practice
BHE	N,N'-Bis(2-hydroxyethyl)ethylenediamine
BHEOX	N,N'-Bis(2-hydroxyethyl)oxamide
BOD	Biological Oxygen Demand
CC	Carbon Capture
ChV	Chronic value
CSIRO	Commonwealth Scientific and Industrial Research Organisation
DEA	Diethanolamine
DEAE	Diethylamine
DEEA	Diethylaminoethanol
DENA	Diethylnitramine
DETA	Diethylenetriamine
DF	Dilution Factor
DGA	Diglycolamine
DIPA	Diisopropanolamine
DMA	Dimethylamine

DMA-NO2	Dimethylnitramine
1DMA-2P	1-(Dimethylamino)-2-propanol
DMAPA	3-Dimethylaminopropylamine
DMMEA	N,N'-Dimethylethanolamine
DMNA	Dimethyl nitramine
DMO	Dimethyloxazolidine
DMPA	Dimethylpropanolamine
DMPDA	Neopentanediamine
DNPZ	Dinitrosopiperazine
DOC	Dissolved organic carbon
DOM	Dissolved organic matter
DREAM	Dose Related Risk and Effects Assessment Model
EA	Ethylamine
EAE	2-Ethylaminoethanol
EC	European Commission
EC ₅₀	Effect concentration with 50% effect
ECHA	European Chemical Agency
EDA	Ethylenediamine
EIF	Environmental Impact Factor
EPA	Environmental Protection Agency
EPI	Estimation Progress Interface
ERA	Environmental Risk Assessment
EtOH-Piper	1-(2-Hydroxyethyl)piperidine
EtOH-Pyrrol	1-(2-Hydroxyethyl)pyrrolidine
EtOH-PZ	1-(2-Hydroxyethyl)piperazine
EU	European Union
FA	Formamide
FW	Freshwater
GLP	Good Laboratory Practice
Glyc	Glycine
HC _x	Hazardous Concentration of x percentile
HEA	N-(2-Hydroxyethyl)acetamide
HEED	N-(2-Hydroxyethyl)ethylenediamine
HEF	N-(2-Hydroxyethyl)formamide
HeGly	N-(2-Hydroxyethyl)glycine

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HEHEAA	Hydroxyethylamino acetamide
HEI	N-(2-Hydroxyethyl)imidazole
HEIA	N-(2-Hydroxyethyl)imidazolidinone
HEPD	1-Hydroxyethane-1,1-phosphonic acid
HEPO	4-(2-Hydroxyethyl)piperazinone
HPLC	high performance liquid chromatography
HSE	Health Safety Environment
ISO	International Organisation for Standardisation
LC ₅₀	Lethal concentration with 50% lethality
LOEC	Lowest observed effect concentration
Log K _{oc}	Soil adsorption partition coefficient
Log K _{ow}	Octanol water partition coefficient
LS-MS	Liquid Chromatography – Mass Spectrometry
MAPA	1-Amino-1-methylaminopropane
MDEA	N-Methyldiethanolamine
MEA	2-Ethanolamine
MEA-NO ₂	Monoethanolnitramine
MeAMP	2-Methyl-2-(methylamino)propane-1-ol
MIPA	1-Amino-2-propanol
MMA	Ethylamine
MMEA	2-Methylaminoethanol
MNA	Methyl nitramine
Morph	Morpholine
NDBA	Nitrosodi- <i>n</i> -butylamine
NDEA	Nitrosodiethylamine
NDELA	Nitrosodiethanolamine
NDMA	Nitrosodimethylamine
NDPA	Nitrosodi- <i>n</i> -propylamine
NMEA	Nitrosomethylethylamine
NMOR	Nitrosomorpholine
NO-HeGly	Nitroso(2-Hydroxyethyl)glycine
NOEC	No observed effect concentration
NOM	Natural organic matter
NPip	Nitrosopiperidine
NPyr	Nitrosopyrrolidine

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NPz	Nitrosopiperazine
OECD	Organisation for Economic Co-operation and Development
OSPAR	Oslo Paris Convention
PAH	Polycyclic aromatic hydrocarbons
PBT	Persistence-Bioaccumulation-Toxicity
PDA	Polydopamine
PEC	Predicted Environmental Concentration
PETA	3-(2-Aminoethyl)aminopropylamine
Piper	Piperidine
2-PiperEtOH	2-piperidineethanol
PNEC	Predicted No-Effect Concentration
ppmV	parts per million by volume
Pyrrol	Pyrrolidine
PZ	Piperazine
Pz-NO ₂	Nitropiperazine
QA	Quality Assurance
(Q)SAR	(Quantitative) Structure Activity Relationship
RBA	Risk-based approach
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
Sarc	Sarcosine
Spermid	N-(3-aminopropyl)1,4-utanediamine
Spermin	N,NN,N'-Bis(3-aminopropyl)-1,4-butanediamine
SRC	Syracuse Research Composition
SSD	Species Sensitivity Distribution
Sulfolane	Tetrahydrothiophenedioxide
SW	Seawater
STP	Sewage Treatment Plant
t _{1/2}	Half-life
TBAB	Tetrabutylammonium
TBEA	N-tert-Butylethanolamine
TCM	Technology Centre Mongstad
TEA	Triethylamine
TGD	Technical Guidance Document
TMBPA	i-[3-(Dimethylamino)propyl]-N,N'-dimethyl-1,3-propanediamine
TMDPA	Tetra-N-methyl-propanedioldiamine



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TONO	Total Nitrosamine
TU	Toxic Unit
UVCB	Unknown or Variable Composition, complex reaction products or biological material
UV-VIS	Ultraviolet visible
vPvB	Very Persistent, very Bioaccumulative
WET	Whole Effluent Toxicity
WFD	Water Framework Directive
Φ	Quantum yields

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1 Executive Summary

This report describes and reviews the principles and methodologies of environmental risk assessment (ERA), including underlying laboratory methods to address persistence (P) bioaccumulation (B) and ecotoxicity (T) of chemicals. There is a strong international focus to avoid the release of PBT compounds in the environment. In this report, internationally approved criteria for defining PBT compounds have been used to classify amines, solvents and their degradation products. The review provided here aims to outline the environmental impacts, characterise the effects from amine-based CO₂ capture plant emissions and support the corresponding risk assessment on the aquatic environment.

The report addresses the following aims and objectives:

- Describes environmental fate processes, such as degradation, photolysis-hydrolysis and presents substance specific partition coefficients, which can influence the amine concentrations in the aquatic environment.
- Provides a classification of potential solvents and degradation products from post-combustion capture facilities.
- Introduces the risk-based approach used in SCOPE, namely 1) to screen emissions for P, B and/or T potential, 2) assess if predicted environmental concentrations are higher than the toxicity thresholds and 3) establish best Available Techniques (BAT) and best environment practice (BEP) of emissions.
- Collect and compile available and reliable data on degradation, bioaccumulation and ecotoxicity of amines, solvents and degradation products relevant for carbon capture technologies. Summarise information from well-grounded databases, such as a SAR database (EPI Suite), and highlight key knowledge gaps.
- Describe the use of assessment factors and mixture models in ERA is described, discussed and tested, and Predicted No-Effect Environmental concentrations (PNECs) for several amines, solvents and degradation products are presented. Based on this, the risk of emissions of potential PBTs are addressed providing a better understanding of potential environmental risks of discharges and to support future ERA processes related to carbon capture.

This report, therefore, represents a basis for regulatory recommendations for harmonising frameworks, emission level thresholds, operational guidelines, and environmental risk management strategies. The data collected and summarised in this report, relates to the fate and effects of amine-based solvents and their degradation products. It will provide input to the environmental risk assessment modelling work for amines and their degradation products and contribute to development of environmental quality standards for emissions from amine-based absorption plants.

The key conclusions from this review are as follows:


- According to PBT criteria, most solvent chemicals (amines), including MEA and PZ, can be considered readily biodegradable, non-bioaccumulative and non-toxic.
- Primary and secondary amino and hydroxyl groups are more degradable than tertiary amines and compounds containing quaternary carbon.

- Due to limited ecotoxicity data, especially chronic data, PNECs for amines are derived using large assessment factors (typically 1,000). More data would warrant SSD estimations, potentially reducing PNECs significantly.
- Based on available acute PNEC values, derived from SAR data, acute ecotoxicity for degradation products is higher than for the solvents; and although, none of the solvent candidates are considered to be toxic, the EC50 values for piperidine and pyrrolidine are 200-300 higher than the threshold level.
- Additivity may be used to explain mixture toxicity of amines in binary mixtures, but more complex emissions need to monitor and take into account contribution from degradation products.
- The Whole Effluent Toxicity together with the PBT assessment are recommended as tier-based approach for the RBA of produced waters.
- In aquatic systems, nitrosamines, while resistant to hydrolysis in water at various pH, degrade rapidly by photolysis under natural sunlight although the degradation rate can be significantly impacted by normal environmental concentrations of NOM. Degradation will decrease with increasing depth in the water column and be limited when nitrosamines are rapidly transported to environmental compartments where there is little or no light penetration (e.g., deeper waters and groundwater).
- Attention should be paid at the environmental fate of nitrosamines during winter periods (low temperatures and short days); The half-lives of nitrosamines are estimated to be higher in such conditions, as compared to summer.
- Photolysis is a particularly important pathway for the degradation of nitrosamines; pH effect on the UV photolysis of different N-nitrosamines shows strong photolabilities in acidic solution, while increasing DOC concentration leads to a decrease in the photodecay rate of nitrosamines. Nitramines, on the other hand, do not degrade by photolysis.
- Nitrosamines are susceptible to photolytic degradation at two absorption bands, with peaks at 230 and 330 nm wavelengths.
- Although nitramines exhibit resistance towards photodegradation, they are formed in sufficiently low quantities and disperse quickly enough that they will most likely reach environmental concentrations significantly below limits and they will be less of concern from a toxicological perspective.
- Biodegradation of nitrosamines is shown to be temperature-dependent; with increased biodegradation at higher temperatures; however, it also differs between different nitrosamines. In addition to temperature-dependency, concentration levels and water type seem to play an important role, with biodegradation being faster at lower concentrations and under freshwater conditions.
- Most of the tested nitrosamines and nitramines are reported to be poorly biodegradable and are candidates for persistency.



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- Previous ecotoxicity tests on freshwater phytoplankton and invertebrate species for the CESAR1 solvent (a mixture of AMP and piperazine which is the main focus solvent in the SCOPE project) have shown a higher EC50 (i.e. it less toxic) for invertebrates than phytoplankton.
 - According to US EPA ECOTOX database, nitrosamines are relatively more acutely toxic to phytoplankton than to invertebrates and fish. Both experimental and SAR data indicated that the ecotoxicities of both compound groups were in the order algae > herbivores (Daphnia) > fish.

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2 Introduction

2.1 Principles of environmental risk assessment (ERA)

2.1.1 Hazard and risk assessment

Environmental 'hazard' is defined as the '*inherent property*' of an agent or situation having the *potential to* cause adverse effects when an organism, system, or (sub)population is exposed to that agent'. 'Hazard assessment' is described as 'a process designed to determine the possible adverse effects of an agent or situation to which an organism, system, or (sub)population could be exposed' (IPCS, 2004). The term environmental 'risk' has been defined by the International Programme on Chemical Safety (IPCS) as '*the probability of* an adverse effect in an organism, system, or (sub)population caused *under specified circumstances by exposure* to an agent', while 'Risk assessment' is described as 'a process intended to calculate or estimate the risk to a given target organism, system, or (sub)population, including the identification of attendant uncertainties, following exposure to a particular agent, taking into account the inherent characteristics of the agent of concern as well as the characteristics of the specific target system' (IPCS, 2004).

The risk assessment process includes four steps (Figure 2.1):

1. Hazard identification: Determining the qualitative nature of the adverse effects by a contaminant
2. Hazard characterisation: Determining the relationship between the dose and the effect (dose–response relationships) and the dose level at which a specific adverse effect can occur to establish an exposure level considered to be acceptable or tolerable.
3. Exposure assessment: Characterising, estimating, measuring and modelling the magnitude, frequency and duration of exposure to a contaminant.
4. Risk characterisation: Integrating the three processes mentioned above to determine the probability of an adverse effect by a contaminant to a population.

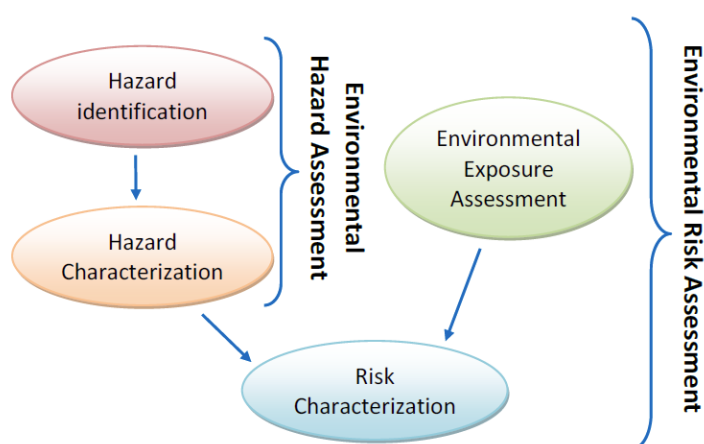



Figure 2.1: The main steps in risk assessment (adopted from OECD).

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If all other external factors are equal, especially the exposures and the organisms subject to them, then the risk is proportional to the hazard. However, all other factors are rarely equal. Risk-based assessment approaches are generally preferred to hazard-based approaches. This is partly due to the recognition that for many environmental issues a level of zero risk is not possible or not necessary for environmental protection, and that a certain level of risk can be accepted. Risk is a combination of hazard and exposure as indicated in Figure 2.1. This implies that there is no direct relation between hazard and risk; a chemical with a high potential hazard may have a low risk if the (probability of) exposure is very low. Conversely, a chemical with a low potential hazard may have a high risk, if the exposure is high.

2.1.2 National and international regulation

Local emissions of pollutants to the environment in Europe are regulated by authorities at the local, national, and international (including EU) levels. Emission permits, based on applications from the owner of the emissions, are normally given by national authorities, but the basis for granting a permit is usually based on international regulations and methods.

At European level, potential health, safety and environmental (HSE) issues relating to emissions are regulated through the European Union Registration, Evaluation, Authorization and Restriction of Chemicals (EU REACH) regulations, the Oslo Paris Convention (OSPAR) and the European Water Framework Directive (WFD). While the EU REACH regulates the European production and import of chemicals based on HSE criteria, OSPAR advise on the offshore use and discharges of chemicals and effluents, while the WFD seeks to improve the quality of the European waterways and estuaries by reductions of potentially harmful chemicals and effluents.

National authorities have mainly focused on discharges of substances of concern, related to potential health or environmental effects, like emissions of nitrosamines and nitramines from amine-based carbon capture facilities. However, in recent years, impacts of the complete discharges/emissions to the environment have gained more attention by national authorities and by international regulators, exemplified by the OSPAR guidelines for risk-based approach, prescribing that the risk of offshore produced water emissions can be characterised based on Whole Effluent Toxicity (WET) as an alternative to a substance-based approach (OSPAR, 2021). However, WET guidelines have not yet been developed for emissions to air.

Emissions to outdoor air are regulated by the EU Directives, namely 2008/50/EC on ambient air quality and cleaner air for Europe (EC, 2008) and 2004/107/EC on heavy metals and PAH in ambient air (EC, 2004). These regulations concern the discharge sources of suspended dust, NO_x and NO₂, SO₂, heavy metals (Pb, As, Cd, Ni, Hg), benzene, benzo[a]pyrene (as PAH indicator), CO and O₃.

2.2 Environmental risk assessment (ERA) methods

As described above, environmental risk assessment (ERA) combines hazard assessment and characterisation with exposure and risk characterisation. In practice, this may be determined as the relation between the environmental concentration of a pollutant and the concentrations associated with adverse effects. The terms predicted environmental concentration (PEC) and predicted no-effect

concentration (PNEC) is used in this context. Risk is associated with a PEC/PNEC >1, meaning that the environmental concentration is higher than the lower concentration suspected to cause harm.

2.2.1 Determinations of PEC and PNEC

PEC represents the predicted environmental concentration of a substance. Emissions to air introduce highly complex processes affecting several environmental compartments (Figure 2.2). Measurements of environmental concentrations may be performed at the source (stack), and if substances accumulate and persist in one of several compartments in a local environment. However, environmental modelling tools will be required to predict air dispersion, fate processes and precipitation. Precipitated material will be subject to further dilutions and fate processes.

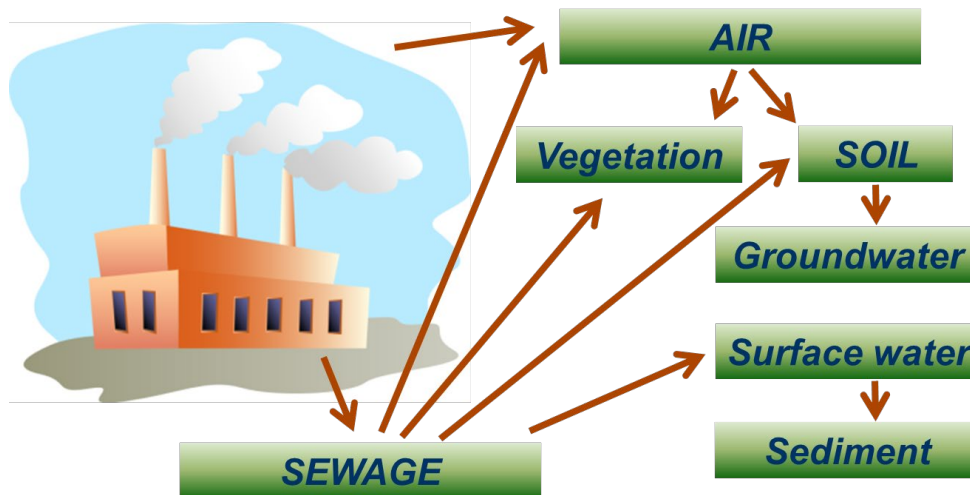


Figure 2.2: Local relevant emission and distribution routes. The figure is adopted from the EU Technical Guidance Document (EC, 2003).

There are many environmental fate processes which can significantly affect the concentration of a chemical released to the environment. In brief, these include (EC, 2003):

- Partition coefficients
 - adsorption to aerosol particles,
 - volatilisation (partitioning between air and water),
 - adsorption/desorption (partitioning between solids and water in soil, sediment and suspended matter).


- Abiotic and biotic degradation processes
 - photochemical reactions in the atmosphere,
 - photolysis in water ground surface,
 - hydrolysis,
 - biodegradation in a sewage treatment plant,
 - biodegradation in surface water, sediment and soil.

PNECs are determined based on the ecotoxicological properties of a substance, i.e., toxicity thresholds or endpoint values after defined periods of exposure. While PECs are described for an emission including multiple substances, PNECs are usually provided thresholds for single substances. The PNECs can be determined by one or several bioassays, representing different trophic levels (levels in a food chain) or by single bioassays. Bioassays may be performed as mortality tests (acute tests) or as chronic tests (subacute tests). When toxicity threshold data from several bioassays are available, the data from the most sensitive assay (organism) should be used. For precautionary purposes, toxicity thresholds are divided by an assessment factor, as shown in Table 2.1. Toxicity thresholds, or endpoint values, from these tests are given as LC50 or EC50, representing the concentration of a substance causing 50 % mortality or inhibition of the test organisms (compared to a control group) and are usually obtained from short-term tests (typically 48-96 hours). NOEC (No Observed Effect Concentration) is the highest tested concentration for which there is no statistically significant difference in effect compared to the control group. NOECs are usually obtained from long-term ecotoxicity studies (chronic tests) typically measuring effects of contaminants on growth or reproduction. In some studies, only LOEC (lowest observed effect concentration) can be obtained, in which case NOEC can be calculated as LOEC/2. Effect concentration x (ECx) is the concentrations at which x % (10% for EC10) effect is observed or derived statistically when compared to the control group. It is usually obtained from long-term ecotoxicity studies. The assessment factors will be high when only short-term (LC50/EC50) tests are available but reduced if long-term tests and several species are included (Table 2.1). A species sensitivity distribution (SSD) approach may also be used and has become increasingly used in the European Union and the United States. SSD is a statistical approach used to estimate either the concentration of a chemical that is hazardous to no more than x% of all species (the HCx) or the proportion of species potentially affected by a given concentration of a chemical. Typically, a HC5 (where no more than 5% of species is affected, estimated from multi-species toxicity thresholds' data) is used and then divided by an AF to derive the PNEC (Versteeg et al., 1999).

Table 2.1: Assessment factors used to derive a PNEC in an aquatic environment (EC, 2003).

Available data	Assessment factor
At least one short-term L(E)C50 from each of three trophic levels of the base-set (fish, Daphnia and algae)	1,000
One long-term NOEC (either fish or Daphnia)	100
Two long-term NOECs from species representing two trophic levels (fish and/or Daphnia and/or algae)	50
Long-term NOECs from at least three species (normally fish, Daphnia and algae) representing three trophic levels	10
Species sensitivity distribution (SSD) method	5-1
	Reviewed on a case-by-case basis
Field data or model ecosystems	Reviewed on a case-by-case basis

If only toxicity data from one acute short-term test are available for a substance, an assessment factor of 1,000 is therefore used to provide a PNEC, and a mortality concentration (LC50) of 100 mg l⁻¹ will result in a PNEC of 0.1 mg l⁻¹. Such large assessment factors have been shown to overestimate chronic toxicity as several reports have significantly lower acute-to-chronic-ratios (ACR) for several species, ranging 1.2 – 23 for petrogenic compounds (McGrath and Di Toro, 2009). Ahlers et al (2006) reported median ACRs for

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fish, daphnids and algae to be 10.5, 7.0 and 5.4, respectively, for a range of industrial chemicals, but also reported that ACRs can vary significantly for different species, and the highest ACR they found was 4,400. Kenaga (1982) also found a very large range of ACRs (1–18,100), and pesticides and metals showed the highest values, whereas 93% of the industrial chemicals had ACRs of less than 25.

2.2.2 Technical Guidance Document – simplified environmental risk assessment

The EU Technical Guidance Document (EC, 2003) describes simplified screening methods determinations of risk assessment of emissions to different compartments (Figure 2.2). While hazard assessment is based on ecotoxicity data and PNEC determinations (Table 2.1), more elaborate methods are used to determine PECs for the different compartments. A PEC for the atmospheric compartment includes local concentration in air during emission episode, annual average local concentration in air, and total deposition flux (annual average). Since the Technical Guidance Document (TGD) is a screening tool, some standard assumptions are made, including a source height 10 meter and estimated concentration in air at a distance of 100 m from the point source (PEC_{local}), representing the average distance between the emission source and the facility border of an industrial site. For the calculation of the PEC_{local} for air, both emission from the point source and the emission from a sewage treatment plant (STP) as possible evaporation is taken into account, the STP is assumed as a point source and the concentration of the substance is calculated at a 100 m distance from the STP emission. Regional concentration in air can also be derived from information given in the TGD.

For the determination of deposition flux the following input data are required: Vapour pressure and Henry's Law constant. Based on the input data and calculations the predicted environmental concentration 100 m from emission source (PEC_{local}) and the average deposition flux within a radius of 1,000 m from the emission source are determined. The latter information is used further as input data for the calculations of PEC for soil. PEC_{local} for the soil compartment is given both for application of sewage sludge in agriculture and for dry and wet deposition from the air compartment. The PEC in agricultural soil is used as a starting point for risk characterisation of terrestrial ecosystems and as a starting point for the calculation of indirect human exposure via crops and cattle products.

The predicted environmental concentration in groundwater is simply derived directly from the concentrations in soil porewater, while the source for surface water is the STP. If no emission of a substance is expected from the STP, the determination of the PEC for the aquatic compartment may be ignored, according to TGD. The PEC for the sediment is derived by using input data from the aquatic compartment, assuming an equilibrium between the water and sediment.

Local relevant emission and distribution routes are summarised in Figure 2.3, while input and output data and calculations are shown in **Appendix 1**.

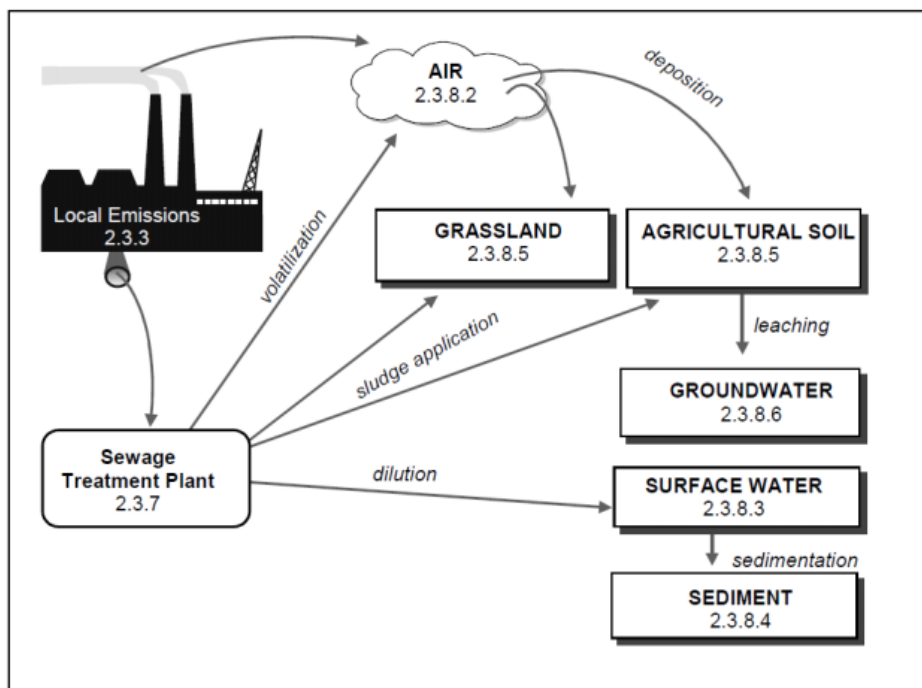



Figure 2.3: Local relevant emission and distribution routes (EC, 2003).

2.2.3 Persistence, bioaccumulation and toxicity (PBT)

From a risk perspective it is important to identify so-called PBT substances, i.e. substances associated with persistence, bioaccumulation and/or toxicity, or vPvB (very persistent and very bioaccumulative) substances. A PBT substance will be available for exposure over long periods, with long exposure periods and the ability to accumulate in the food chain. According to the European Chemical Agency (ECHA), the criteria for PBT substances are as shown in Table 2.2.

Table 2.2: Criteria for PBT and vPvB chemicals, according to Annex XIII to REACH (ECHA, 2017a).

Property	PBT-criteria (Annex XIII to REACH)	vPvB-criteria
Persistence	$T_{1/2} > 60$ days in marine water $T_{1/2} > 40$ days in freshwater/estuarine water $T_{1/2} > 180$ days in marine sediment $T_{1/2} > 120$ days in soil	$T_{1/2} > 60$ days in marine, fresh, or estuarine water $T_{1/2} > 180$ days in marine, fresh, or estuarine sediments $T_{1/2} > 180$ days in soil
Bioaccumulation	$\log PoW > 4.5$ Bioconcentration factor (BCF) $> 2,000$	$\log PoW > 4.5$ Bioconcentration factor (BCF) $> 5,000$
Toxicity	NOEC or LC10 $< 0.01 \text{ mg l}^{-1}$ for marine or freshwater organisms Specific classifications of mammalian toxicity (carcinogenicity, mutagenicity and reproduction inhibition) and chronic toxicity	

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The information used in the PBT/vPvB assessment is divided into two types: screening information, and assessment information. Screening information will include ready or inherent biodegradability tests, octanol-water partitioning coefficient determination and short-term ecotoxicity tests. Substances with ≥ 70 % DOC removal or ≥ 60 % mineralization by respirometric tests (CO_2 accumulation or biochemical oxygen demand), $\log K_{ow} \leq 4.5$ by octanol-water partitioning coefficient determination, and $\text{LC}_{50}/\text{EC}_{50} \geq 0.1 \text{ mg l}^{-1}$ are not to be considered as P, B or T substances. Substances not meeting these criteria are to be considered as potential P, B or T substances (ECHA, 2017a). Assessment information should then be collected for final decisions. P/vP should normally be based on degradation half-life data collected under adequate conditions for the relevant compartment(s) of exposure, B/vB be based on measured data on bioconcentration in aquatic species, and T based on evaluation of the data from human health hazards and/or on no-observed effect concentration(s) (NOECs) or EC10 from long-term toxicity tests with aquatic organisms (ECHA, 2017a).

For substances containing multiple constituents (UVCB-substances, well defined multi-constituent substances and mono-constituent substances with multiple impurities) the substance may be considered PBT if individual amounts ≥ 0.1 % (w/w) or transformation/degradation products with PBT/vPvB properties in relevant amounts are being generated. If emissions contain one or several components with PBT properties, or transformation/degradation products with these properties are formed, the substance should be subject to emission and risk characterisation. By emission characterisation, the amounts and rates of the PBT/vPvB substance should be estimated, as well as the likely routes by which humans and the environment are exposed to the substance. The objective of a risk characterisation will then be to recommend actions to which minimise exposures and emissions to humans and the environment throughout the lifecycle of the substance. A flowsheet for the ECHA PBT assessment process is described in Figure 2.4.

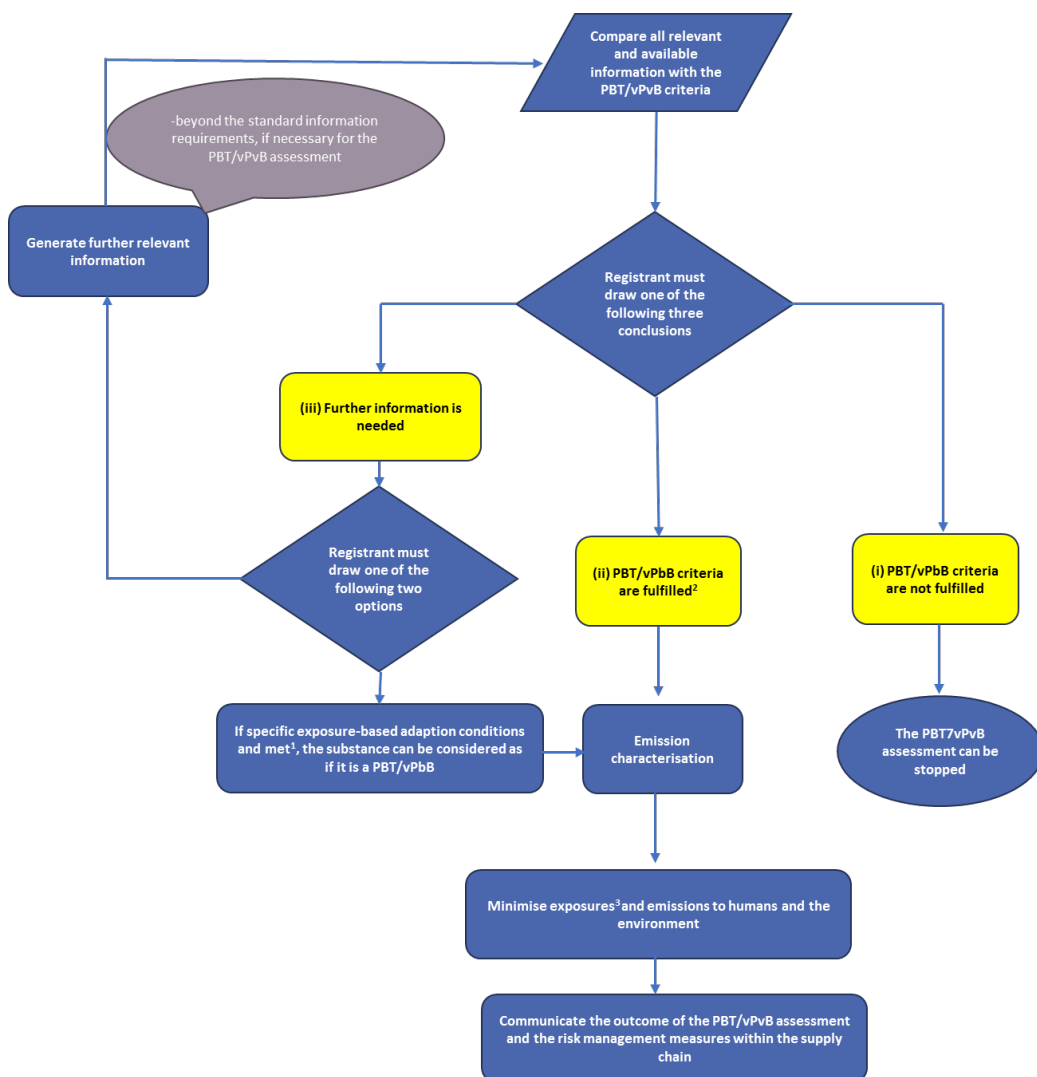


Figure 2.4: Overview of the PBT/vPvB assessment process for the registrant (ECHA, 2017a).

2.2.4 Mixture toxicity

While most hazard and risk assessment methods are designed for single compounds, many substances, and particularly emissions, are released with multiple components, each with different fate and ecotoxicological properties. Tools have been developed for estimation of toxic responses for multi-constituent substances, based on the toxicological properties of the individual constituents. One such tool is the additive toxicity determination (French-McCay, 2002):

$$LC50_{\text{mix}} = \frac{1}{\sum \frac{F_i}{LC50_i}},$$

where $LC50_{\text{mix}}$ is the total toxicity of the mixture, F_i is fractional concentration, and $LC50_i$ is LC50 or EC50 of the individual substances i .

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In theory, the ecotoxicity of two or more chemicals may be the sum of the toxicities of the individual components. This is the concept of additive toxicity used for instance for the determination of complex mixtures like petroleum (French-McCay, 2002). If the concept is valid, the toxicity of the mixture should be similar to the sum of the calculated toxicity of the individual components. If the concept is not valid this may be explained by synergistic or antagonistic interactions of the individual compounds.

The toxic unit (TU) approach may also be used for mixtures and to identify if constituents have additive, synergistic or antagonistic effects. According to the TU model (Norwood et al., 2003; Playle, 2004), in a mixture, the relevant endpoint of each constituent (e.g., EC50-value, 50% mortality) is given a value of TU=1. If two constituents with known endpoint values are mixed in equimolar concentrations, the mixture of these should result in a TU=1 if the mixture is strictly additive (50% mortality), while a TU<1 describes antagonistic effects (effects less than additive; less than 50% mortality) and a TU>1 describes synergistic effects (effects greater than additive; more than 50% mortality), as shown in Figure 2.5.

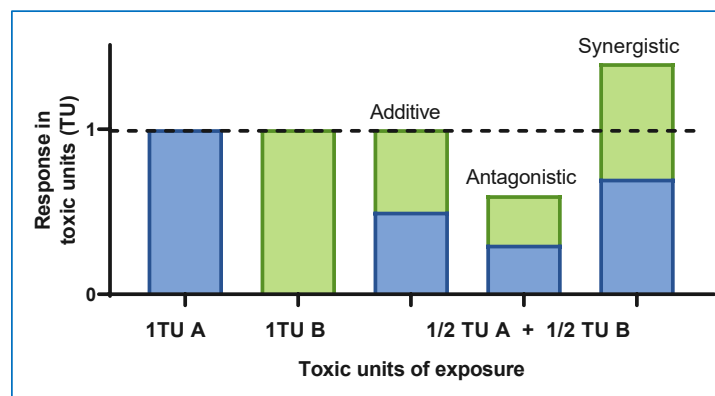


Figure 2.5: Theoretical models for assessing the interaction of chemicals in mixture. The combined effects of two chemicals (A, B) in a toxicity test quantified by expressing the concentration of toxicants A and B in mixture as toxic units (Hepditch et al., 2021).

The toxicity of a mixture is a very complex issue and depends on a high number of variables, particularly when the mixture is distributed in different environmental compartments. The different constituents in the mixture may have different properties in relation to the fate processes in the different compartments, including water solubility, particle attachment, degradation processes (hydrolysis, photochemical reactions, biodegradation), and bioaccumulation and biomagnification in organisms and the food chain. For precautionary reasons, regulators are, therefore, often focusing on the constituent(s) in the mixture expected to represent the highest health and/or environmental risk, based on available single constituent information.

2.2.5 Whole effluent toxicity (WET) and risk-based approach (RBA)

The whole effluent toxicity approach (WET) is a system where the toxicity of a complete mixture is tested, often in combination with information provided from the known constituents in the mixture. The composition of complex mixtures and degradation products are often lost, since chemical

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characterisation and quantification tools usually identify and targeted compounds, while non-target compounds may be unnoticed. Using WET methods will, therefore, in theory include the complete sample with all its compounds. The WET technology has been recommended by OSPAR for the risk-based approach (RBA) of produced water from offshore installations in the North Sea. A combination of WET, single substance approach, in combination with PBT assessment, have been suggested as a tier-based approach for RBA of produced water by the UK Department for Business, Energy and Industrial Strategy, as shown in Figure 2.6 (DBEIS, 2020).

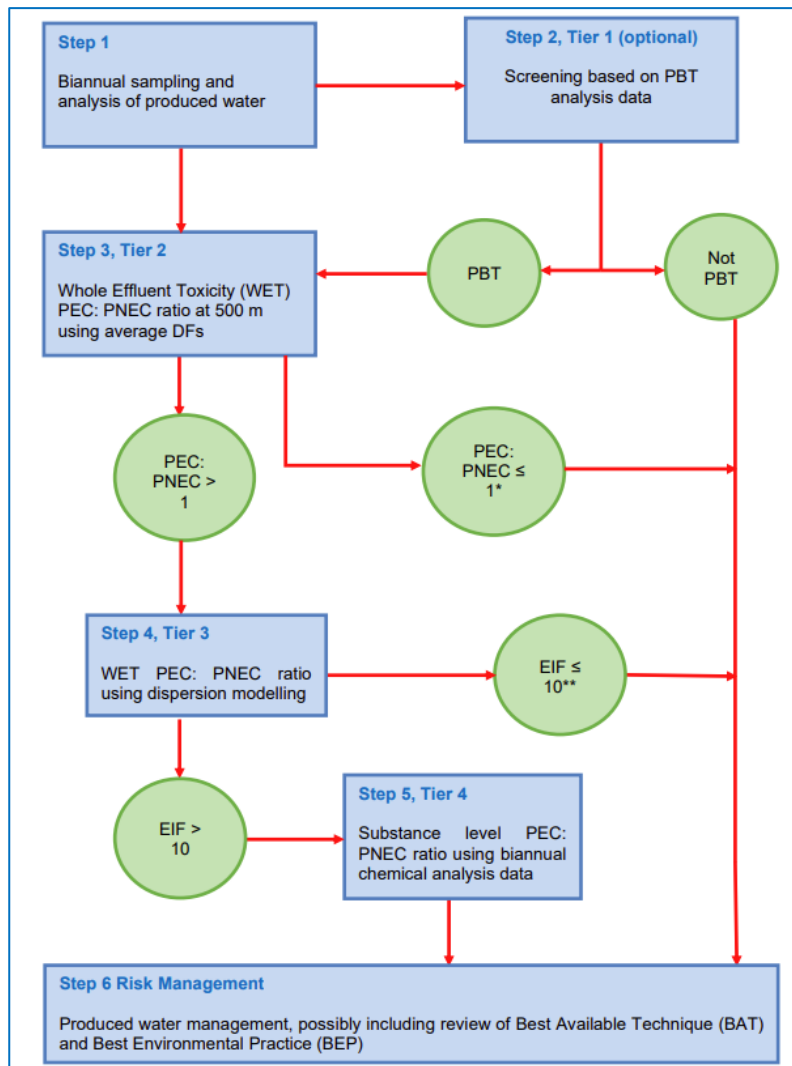


Figure 2.6: The tier-based approach for RBA of produced water from offshore installations (DBEIS, 2020).

Figure 2.6 shows the RBA as described for offshore emissions to seawater based on a combination of monitoring of the emissions. WET is determined by testing the produced water in ecotoxicity tests using marine test organisms that represent three different trophic levels (Tier 2). Produced water PEC

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determinations at a defined distance from the emission source (500 m), is determined using an average dilution factor (DF) obtained by dispersion modelling. The PEC/PNEC is then determined (see Table 2.1 for determination of PNEC). If $PEC > PNEC$, a more elaborate WET method is used (Tier 3), involving modelling of produced water discharges and identifying whether the PEC/PNEC ratio is >1 within the modelled volume and/or area. The Tier 3 modelling indicates whether the time averaged PEC/PNEC ratio for the whole effluent is >1 within the selected volume and/or area during the modelling period. The results, therefore, reflect the worst-case scenario. An environmental impact factor (EIF) is determined, using the Dose-related Risk and Effects Assessment Model (DREAM) model (Reed and Hetland, 2002). If $PEC/PNEC > 1$, a risk is considered for 5% of the most sensitive species, and if 10^5 m^3 water is considered to have this risk, this represents an $EIF = 1$. If 10 times larger water volumes have a $PEC/PNEC > 1$, this represents an EIF of 10, which is considered to represent a low environmental risk. If the $EIF > 10$, modelling of individual components of the produced water discharge should be performed to determine the fate and contribution to the total risk of the specific components in the produced water stream (Tier 4 in Figure 2.6). For produced water emissions with $EIF > 10$, risk-reducing efforts should be made to obtain an $EIF \leq 1$, including a) technical measures like redesign of the applied processes, b) substitution of chemicals, c) application of closed systems (e.g. re-injection of produced water), d) produced water treatment (end-of-pipe techniques), and e) organisational measures such as management systems in place, like training, instructions, procedures and reporting (DBEIS, 2020).

Although the RBA methods, including the WET methods are currently designed only for direct emissions to water environments, important elements from these methods should also be relevant for emissions to air, particularly if some of the emissions eventually end up in aquatic systems.

2.3 Degradation methods

Degradation tests are performed to determine the potential persistence of substances, either by abiotic (hydrolysis or photodegradation) or by biological (biodegradation) processes. Standardised methods are described in the OECD Guidelines for the Testing of Chemicals, section 1, Physical-Chemical properties (OECD, 2023a), and in Section 3, Environmental fate and behaviour (OECD, 2023b).

Degradation data may be predicted by quantitative structure-activity relationships (QSAR). QSAR is a computational or mathematical modelling method used to estimate the relationships between the structural properties of a substance and its biological activities. The system is based on data from numerous tests describing the biological activity (e.g., biodegradation), in which rules are made to predict the biological activities of structurally-closely related chemicals. A well-known structure-activity relationship (SAR) database is the Estimation Programs Interface (EPI) Suite™ developed by the US Environmental Protection Agency's (EPA) and Syracuse Research Corporation (SRC). This SAR system includes physical-chemical, biodegradation, and ecotoxicity databases for organic chemicals. Certain processes are crucial for the persistence of nitrosamines in the environment and especially in fresh water, for the potential exposure period to man through direct and indirect uptake. Such elements include hydrolysis, photolytic degradation, biodegradation and bioaccumulation, under oxic and anoxic conditions.

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2.3.1 Hydrolysis

The standard hydrolysis method describes the physical transformation of substances as a function of pH (OECD, 2004a). Substances are tested at pH values normally found in the environment (pH 4 – 9). A preliminary test (Tier 1) is performed by incubation of the substance at pH 4, 7, and 9 at 50°C for 5 days. If the substance is unstable at some of the pH levels, an extended test (Tier 2) is performed (up to 30 days) and an identification of the degradation products may be performed (Tier 3).


2.3.2 Photodegradation

Photodegradation describes the degradation of substances by sunlight/daylight. The OECD 301 test method describes the determination of the ultraviolet-visible (UV-VIS) absorption spectrum of a chemical compound to have some indication of the wavelengths at which the compounds may be susceptible to photochemical degradation (OECD, 1981). A photodegradation test in water is described in the OECD test method 316 (OECD, 2008a). This is a tier-based procedure which first screens if the test substance is susceptible to photodegradation in artificial sunlight, and if so, a rate constant and half-life is determined experimentally, as well as the transformation pathway and the identities, concentrations, and rate of formation and decline of major transformation products.

2.3.3 Biodegradation

Biodegradation tests can be performed as screening tests or as simulation tests, and methods for both levels of tests are described in the OECD Guidelines for the Testing of Chemicals, section 3, Environmental fate and behaviour (OECD, 1992a). Biodegradation potentials are screened by the OECD test method 301 Ready biodegradability. This test is performed in a freshwater medium propagated with extra inoculum (bacterial source) from sludge, wastewater treatment plant waste, or soil. The test substance at a high concentration is incubated with the inoculum and water amended with essential added macronutrients for 1 to 2 months, and ultimate biodegradation measured as CO₂ accumulation or biochemical oxygen demand (BOD). If ultimate biodegradation is ≥ 60% after 28 days, the substance is judged to be readily biodegradable. However, if ultimate biodegradation is < 60%, biodegradation is not ruled out, and extended tests can be performed, including enhanced ready biodegradation tests (e.g. extended incubation times and/or increased test volumes) and simulation tests. Simulation tests are performed in natural non-amended water with low test substance concentration, often requiring the use of radiolabelled substances (14C-labelled). Examples of simulation tests are the OECD 308 (aerobic-anaerobic simulation test in sediment-water and 309 test (aerobic simulation test in water) methods, where test substances are applied in two concentrations (e.g. 1-10 µg l⁻¹ and 100 µg l⁻¹) and incubations performed at ambient temperatures (temperature at the water source) or at 20-25°C for 60 days. Ultimate biodegradation when 14C-labelled substances are used are performed by trapping of ¹⁴CO₂ in an alkali-trap (OECD, 2004b, 2002).

For determination of biodegradability in seawater, the OECD test method 306 describes ultimate biodegradation in seawater, using natural seawater as inoculum (OECD, 1992b). This test very much resembles the OECD301 test method and, therefore, may be used to determine the ready biodegradability of substances in seawater. However, since seawater is used as inoculum, the bacterial concentrations are low compared to the OECD301 test method, where the water has been propagated with extra inoculum (OECD, 1992a). A revision of the OECD 306 test method has, therefore, been

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suggested with extra inoculum concentrations achieved by concentration of seawater bacterial concentrations by tangential flow filtration (Ott et al., 2020).

An overview of degradation data for regulatory use as part of risk characterisation of substances is shown in Figure 2.7.

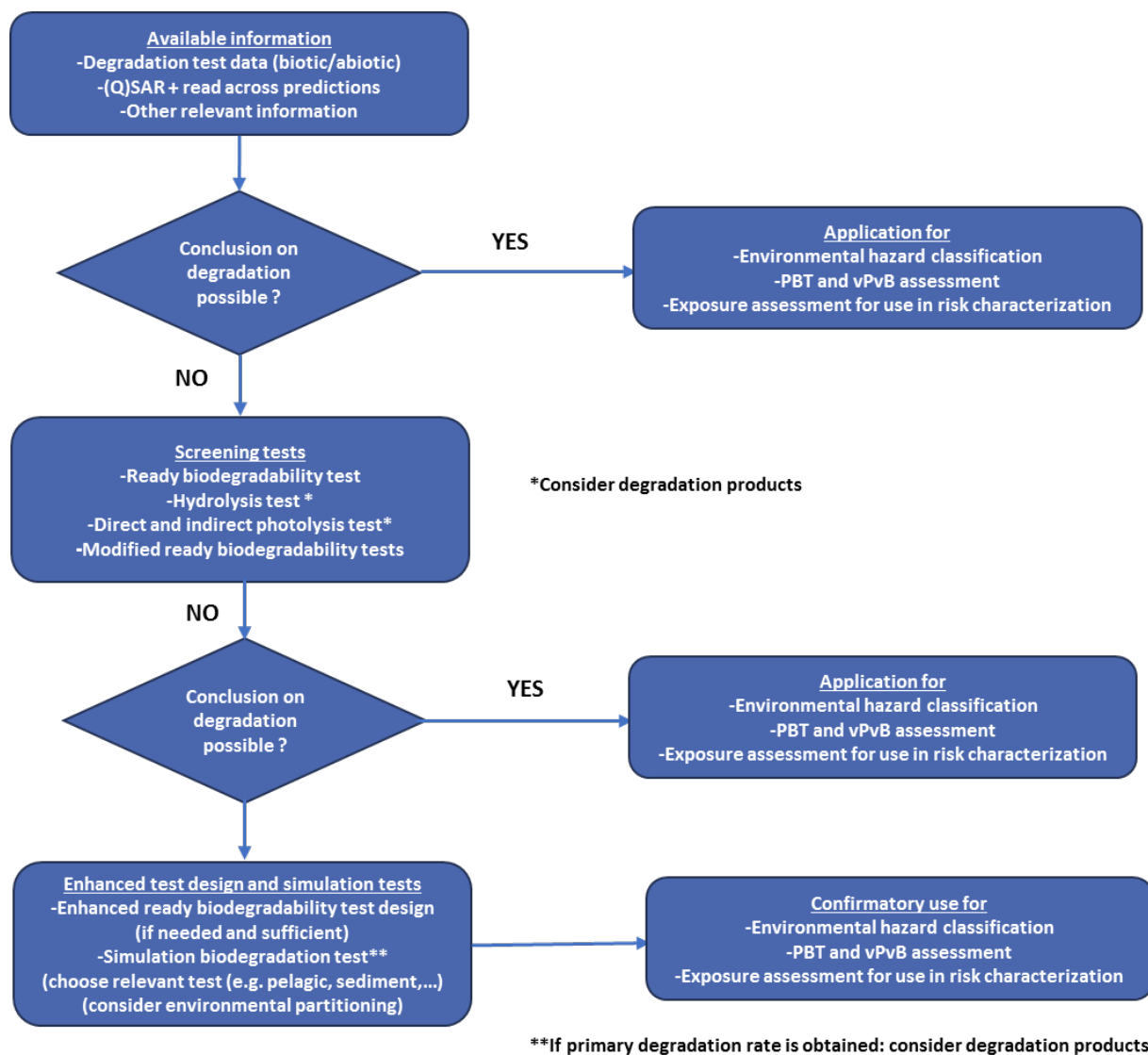


Figure 2.7: Overview decision scheme on degradation for the three regulatory needs Environmental hazard, PBT/vPvB assessment and exposure assessment for use in risk characterization (ECHA, 2017a).

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2.4 Bioaccumulation

Bioaccumulation describes the potential uptake and accumulation of substances in fatty tissues. Bioaccumulation is determined as the distribution of the substance between two immiscible phases as a screening method, or as the bioconcentration factor (BCF) between animal tissues and the surrounding environment (i.e., the water phase for pelagic organisms and the sediment or soil phase for sediment and soil organisms). Sections 1 and 3 of the OECD Guidelines also include methods for determination of bioaccumulation, which refer to the uptake and accumulation of substances in fatty tissues.

2.4.1 Octanol-water coefficients

As a screening for potential bioaccumulation properties, the water-octanol partition coefficient is determined, by determination of the distribution of substances between a solid phase containing long hydrocarbon chains chemically bound onto silica (immobile phase) and a mobile water phase. The substances are retained in the column in proportion to their hydrocarbon-water partition coefficient, with hydrophilic chemicals eluted first and lipophilic chemicals last, and the partition coefficient ($\log P_{ow}$) of the test substance is determined. The high performance liquid chromatography (HPLC) method covers a partition coefficient range of $\log P_{ow}$ 0 (low) to 6 (high) $\log P_{ow}$ (OECD, 2022).

2.4.2 Bioconcentration factors – bioassays

Bioconcentration factors (BCFs) are determined in bioassays with pelagic, sediment or soil species, as described in section 3 in the OECD Guidelines. Test methods for determinations of BCFs in fish and sediment or terrestrial oligochaetes are described by OECD (OECD, 2012, 2008b). The tests are performed in two periods; one exposure period where the organisms are exposed to the substance at one or more concentrations (often 28 days), and one post-exposure period where the organisms are moved to a clean system without the test substance (depuration). BCFs are then determined as the ratio of concentration in the organisms (fish or oligochaetes) and in the surrounding environment (water, sediment or soil).

2.5 Ecotoxicity methods

Ecotoxicity methods are used to determine the hazard of pollutants, either as mixtures, or as single components. For regulatory purposes, standardised methods are used to determine acute or chronic toxicity to species representing different trophic levels. Standardised ecotoxicity tests are described for aquatic (freshwater and marine), soil and air habitats, but tests with aquatic species are by far most used. Tests with soil species and with air species (insects or birds) are more complex to perform and may result in more unreliable data than with aquatic species. Tests with aquatic species can further be separated in the species with free water and sediments as their main habitats. A comprehensive collection of standardised ecotoxicity tests is given in the OECD Guidelines for the Testing of Chemicals, Section 2, Effects on biotic systems (OECD, 2023c).

Short-term acute tests are usually performed to determine lethal or immobilising concentrations of pollutants, to determine endpoints, like LC50/EC50 or LC10/EC10, i.e., concentrations which are lethal or inhibit 50% or 10% of the population when compared to non-exposed control cultures. These data are then used to determine PNECs, as described in Table 2.1. Since most species have different sensitivities to pollutants over different life-stages, it is relevant to perform the ecotoxicity tests using the most

sensitive stages. Chronic tests are used to determine endpoints that are not lethal but inhibit some processes that affects the population on a more long-term period. The most common example of chronic endpoints is reproduction, and these tests, therefore, need to be performed over several generations.

2.5.1 Acute ecotoxicity

An acute toxicity test is conducted to obtain information concerning the immediate effects on test organisms of a short-term exposure (typically 24-96 h) to a test material under specific experimental conditions. Immobilised or dead test animals are counted in serially diluted exposure solutions, and statistical methods are used to assess dose-response relationships and estimate toxicity thresholds, like LC50. There are standardised test procedures available from OECD, ISO and ASTM for different species. For aquatic toxicity, the most widely used acute toxicity tests are OECD Guideline 201 (Freshwater Alga and Cyanobacteria, Growth Inhibition Test), OECD Guideline 202 (*Daphnia* sp. Acute Immobilisation Test) and OECD Guideline 203 (Fish, Acute Toxicity Test). Alternative methods to avoid/reduce the use of (juvenile) fish in the interest of animal welfare and efficient use of resources, are recommended, e.g., using the fish embryo test, fish cell lines and QSARs. Species mentioned in the OECD guideline are all warm freshwater species including zebrafish (*Danio rerio*), fathead minnow (*Pimephales promelas*), carp (*Cyprinus carpio*), Japanese medaka (*Oryzias latipes*), guppy (*Poecilia reticulata*) and bluegill (*Lepomis macrochirus*). The selection of fish species depends on regulatory requirements and on relevant environmental exposure scenarios, so non-model fish species relevant for colder temperatures and estuarine/marine environments may also be used. The same also applies for algae and microcrustacean, where marine alternatives to the green algae *Pseudokirchneriella subcapitata* and the cladoceran *D. magna* are e.g., the *Skeletonema costatum* (marine algae) and *Acartia tonsa* (marine copepod).

Below are given examples of how ecotoxicity tests are performed, using the aquatic species *Daphnia* sp. (water flea) as an example. This is probably the most common aquatic test organism for ecotoxicity tests. *Daphnia* is a genus of small planktonic crustaceans, 0.2–6.0 mm in length living in various aquatic environments ranging from acidic swamps to freshwater lakes and ponds (Figure 2.8).

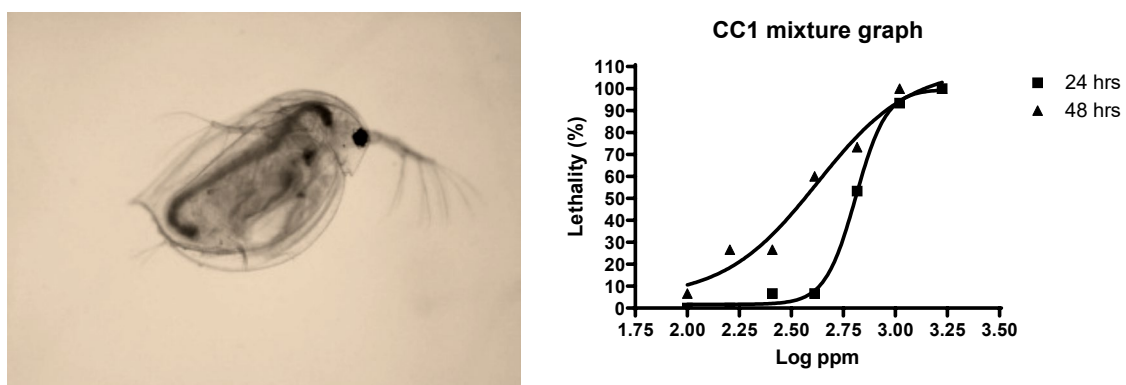


Figure 2.8: Left - A young *Daphnia magna* (photo: Bjørn Henrik Hansen, SINTEF Ocean) and right - a typical inhibition curve used for determination of EC50, using data from testing of CESAR1 (Brakstad et al., 2010).

The *Daphnia* sp. Acute Immobilisation test is described in the OECD Guideline 202 (OECD, 2004c). In brief, a *Daphnia* start culture of females is fed on phytoplankton (algae) at 20-20°C for several generations. Young individuals (neonates/juveniles) are exposed to different concentrations of a test substance (3 replicates) for 48 hours at 20-22°C in a freshwater with added macro-nutrients and vitamins and a solution of trace elements. Control cultures (6 replicates) are included in which the organisms are not exposed to the test substance. The numbers of immobilised organisms in each culture are counted after exposure for 24 and 48 hours, and an inhibition curve prepared to determine EC50, as shown in Figure 2.8B.

2.5.2 Sublethal effects – chronic toxicity

Acute toxicity tests do not provide information about the potential for delayed effects to occur, although post-exposure observations of effects may provide some relevant information. Sub-lethal effects on development and reproductive output are ecologically relevant effects for sublethal or chronic testing. Chronic toxicity tests are longer-term tests that measure the effects of exposure to lower and less acutely toxic concentrations. Chronic toxicity tests assess adverse effects occurring after repeated or continuous contaminant exposure during a significant portion (typically at least 10%) of the life span of the test species. Adverse effects associated with chronic toxicity commonly cover changes in growth, reproduction, or behaviour. Standardised sublethal or chronic tests are available, including copepod early life stage test (ISO, 2015), *Daphnia magna* reproduction test (OECD, 2004c), fish juvenile growth test (OECD, 2000), fish prolonged toxicity test, 14-day (OECD, 1984), fish short term reproduction assay (OECD, 2018) and fish sexual development test (OECD, 2011).

2.6 (Quantitative) structure-activity relationships (Q)SAR

Environmental data like ecotoxicity and biodegradation may be predicted by (quantitative) structure-activity relationships ((Q)SARs). (Q)SARs are computational or mathematical modelling methods used to estimate relationships between the structural properties of a substance and its biological activities and their physical-chemical properties (e.g., water solubility, melting and boiling points, vapour pressure, Henry's Law constant). The system is based on data from numerous tests describing the biological activities, in which correlations/regressions are used to predict the biological activities of structural closely related chemicals. A well-known and easily accessible structure-activity relationship (SAR) database is the Estimation Programs Interface (EPI) Suite™ (EPISUITE) developed by the US Environmental Protection Agency's (EPA) and Syracuse Research Corporation (SRC). This SAR system includes physical-chemical, biodegradation, and ecotoxicity databases for organic chemicals. Ecotoxicity estimations are covered by the ECOSAR module, predicting the acute toxicity (EC50/LC50) of green algae, daphnids and fish, as well as a chronic value (ChV) with these tropic groups. From collections of measured aquatic toxicity values and estimated Kow values, regression equations have been developed for different classes of chemicals. The toxicity values for new chemicals may then be calculated by inserting the estimated Kow into the regression equation and correcting the resultant value for the molecular weight of the compound (Meylan et al., 1996) .

EPI Suite™ can be used to initially screen substances for potential PBT properties, as shown in Table 2.3 (ECHA, 2017a). This system can be used as a pre-screening system when experimental data are not available or inadequate.



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Table 2.3: Screening information for Persistence, Bioaccumulation, and Toxicity, based on the EPISUITE SAR information (ECHA, 2017a).

Property	PBT-criteria (Annex XIII to REACH)	vPvB-criteria
Persistence BOWIN 3 (ultimate biodegradation time)	Ultimate biodegradation timeframe prediction: \geq months (value < 2.25 (to 2.75))	Potentially P or vP
Bioaccumulation Octanol-water partitioning coefficient (experimentally determined or estimated by QSAR)	Log Kow > 4.5	Potentially B or vB (in aquatic organisms)
Toxicity Short-term aquatic toxicity (algae, daphnia, fish)	EC50 or LC50 < 0.01 mg l ⁻¹	EC50 or LC50 < 0.01 mg l ⁻¹

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	Dissemination level	Public

3 Risk assessment in the context of amine-based carbon capture

3.1 Chemicals and degradation products

Potential solvents for amine-based carbon capture (CC) are classified in primary, secondary and tertiary amines, and in alkanolamines, sterically hindered alkanolamines, polyamines, cyclic amines, amino acids, volatile amines and organo-sulphur compounds, as listed in Table 3.1 (Eide-Haugmo et al., 2012).

The degradation products from these solvents may be numerous. In recent years, focus has primarily been on the potentially carcinogenic nitrosamines and nitramines. Other degradation products include aldehydes, ketones, amines, amides and ammonia. Some relevant products are described in Table 3.2. These degradation products are substances which have been detected in CC pilot plants, or may potentially occur as degradation products from different degradation processes (Brakstad et al., 2018; Brakstad et al., 2010; Languille et al., 2021; Morken et al., 2017a; Moser et al., 2020). Several of the degradation products may occur in the solvent, however, may not be present in the emissions, as was shown in recent MEA testing campaigns (Morken et al., 2017a). Importantly, however, there is an inherent uncertainty related to the environmental risk of unknown degradation products for which methods for identification and quantification are not available.


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Table 3.1: Potential CC amine candidates related to group. The amine groups include primary (p), secondary (s) and tertiary (t) alkanolamines (alkanolam), sterically hindered alkanolamines (s-h-alkanolam), polyamines (polyam), cyclic amines (c-am), amino acids (am-ac), volatile amines (vol-am) and organo sulphur (org-sulph) compounds.

Substance group	Substance	Abbr.	Substance group	Substance	Abbr.
p-alkanolam	2-Ethanolamine	MEA	s-polyam	1-Amino-1-methylaminopropane	MAPA
	3-Aminopropanol	AP		Diethylenetriamine	DETA
	4-Amino-1-butanol	AB		3-(2-Aminoethyl)aminopropylamine	PETA
	1-Amino-2-propanol	MIPA		<i>N</i> -(3-aminopropyl)1,4-utanediamine	Spermid
	Dilycolamine	DGA		<i>N,N,N'</i> -Bis(3-aminopropyl)-1,4-butanediamine	Spermin
s-alkanoam	2-Methylaminoethanol	MMEA	t-polyam	1-Amino-1-cyclohexylaminopropane	ACHP
	2-Ethylaminoethanol	EAE		Dimethylaminopropylamine	DMAPA
	Diethanolamine	DEA		Tetra- <i>N</i> -methylpropanedioldiamine	TMDPA
	Diisopropanolamine	DIPA	c-am	<i>i</i> -[3-(Dimethylamino)propyl]- <i>N,N</i> -dimethyl-1,3-propanediamine	TMBPA
	<i>N</i> -(2-Hydroxyethyl)ethylenediamine	AEEA		Piperazine	PZ
	<i>N,N'</i> -Bis(2-hydroxyethyl)ethylenediamine	BHE		1-(2-Hydroxyethyl)piperazine	EtOH-PZ
t-alkanolam	<i>N,N</i> -Dimethylethanolamine	DMMEA	1-(2-Aminoethyl)piperazine	AE-PZ	
	<i>N</i> -methyldiethanolamine	MDEA	Morpholine	Morph	
	Diethylaminoethanol	DEEA	Piperidine	Piper	
	Triethanolamine	TEA	2-piperidineethanol	2-PiperEtOH	
	Dimethylpropanolamine	DMPA	1-(2-Hydroxyethyl)piperidine	EtOH-Piper	
	1-Dimethylamino)-2—propanol	1DMA-2P	Pyrrolidine	Pyrrol	
	1-(2-Hydroxyethyl)pyrrolidone				
s-h-alkanolam	2-Amino-2-methylpropanol	AMP	am-ac	Alanine	Ala
	2-Amino-2-methyl-1,3-propanediol	AMPD		Sarcosine	Sarc
	2-Amino-2-ethyl-1,3-propanediol	AEPD		Glycine	Glyc
	<i>N-tert</i> -Butylethanolamine	TBEA	vol-am	Dimethylamine	DMA
	Tetrabutylammoniumbromide	TBAB		Triethylamine	TeA
p-polyam	Ethylenediamine	EDA	org-sulf	Tetrahydrothiophenedioxide	Sulfolane
	1,3-Propandiamine	PDA			
	Neopentanediamine	DMPDA			

Table 3.2: Potential degradation products of CC amines solvents. The degradation products are grouped in aldehydes, amines, amides, ammonia, nitrosamines and nitramines.

Substance group	Substance	Substance group	Substance
Acids	Acetic acid	Cyclic	Morpholine
	Oxalic acid		4-Acetomorpholine
	Bicine		Imidazole
	1-Hydroxyethane-1,1-phosphonic acid (HEPD)		N-(2-Hydroxyethyl)imidazole (HEI)
	N-(2-hydroxyethyl)glycine (HeGly)		1-(2-Hydroxyethyl)-2-imidazolidinone (HEIA)
Ammonia	Ammonia		Pyrrole
Aldehydes	Formaldehyde		1,1'-(1,3-Phenylene)bis-1H-pyrrole-2,5-dione
	Acetaldehyde		Pyrazine
Alcohols	Ethylene glycol		Methylpyrazine
Ketones	Acetone		Dimethylpyrazine
Nitriles	Acetonitrile		Oxazolidone
Amines	Methylamine		4,4-dimethyloxazolidone
	Dimethylamine		<i>N</i> Nitrosodiethanolamine (NDELA)
	Ethylamine		Nitrosopiperidine (NPIP)
	Diethylamine		Nitrosodiethylamine (NDEA)
	Ethyl-methylamine	Nitrosodimethylamine (NDMA)	
	Propylamine	Nitroso- <i>N</i> -methylethylamine (NMEA)	
	2-Methyl-2-(methylamino)propane-1-ol	Nitrosomorpholine (NMOR)	
	Nitromethane	Nitroso- <i>N</i> -dipropylamine (NDPA)	
	Nitroethane	Nitrosopyrrolidine (NPYR)	
	N-(2-Hydroxyethyl)-ethylenediamine (HEED)	Nitrosopiperazine (NPZ)	
Amides	Formamide	Dinitrosopiperazine (DNPZ)	
	Acetamide	Nitroso(2-hydroxyethyl)glycine (NO-HeGly)	
	N-(2-hydroxyethyl)-formamide (HEF)	Nitramines	
	N-(2-Hydroxyethyl)acetamide (HEA)	Dimethylnitramine (DMNA)	
	Hydroxyethylamino acetamide (HEHEAA)	Ethanolnitramine (MEA-NO ₂)	
Cyclic	N,N'-Bis(2-hydroxyethyl)oxamide (BHEOX)	Methylnitramine (MNA)	
	Piperazine	<i>N</i> -Nitropiperazine (PZ-NO ₂)	
	4-(2-Hydroxyethyl)piperazinone (HEPO)	1-Methyl-2-(nitroamino)-1-propanol (AMP-NO ₂)	
		Diethylnitramine (DENA)	

	Document	Deliverable D3.1
	Issue date	03 Feb 2023
	Dissemination level	Public

4 Ecotoxicity, bioaccumulation and degradation data

4.1 SAR data of solvents and degradation products

In this report we have collected ecotoxicity, bioaccumulation and degradation data for potential solvent and degradation substances. Since experimental data are limited for several of the substances, a set of SAR data have been provided by the EPI Suite™ database, as shown in **Appendix 2**. A number of 49 potential solvent substances and 58 possible degradation products (Table 3.1 and Table 3.2) were screened for degradability, bioaccumulation and ecotoxicity in the SAR system. None of the solvents or degradation products were classified as potential B or T candidates, according to the levels described in Table 2.3. Persistence cannot be determined from these criteria, although 4 solvents and 11 possible degradation products were classified as not readily biodegradable (time factor of weeks to months for ultimate biodegradation). These included the three tertiary polyamines DMAPA, TMPDA and TMBPA, the volatile amine TEA (Table 3.1), eight nitrosamines (NDEA, NDMA, NMEA, NMOR, NDPA, NPYR, NPZ and DNPZ) and two nitramines (DMNA and DENA) (Table 3.2). It must be noted that two of the eleven nitrosamines, three of six nitramines, along four other degradation products included in the data set could not be classified using the EPISUITE system (**Appendix 2**).

PNEC values determined from the SAR data indicates the acute ecotoxicities of the degradation products were higher than for the solvents, as it was noted that median PNEC values were lower for the degradation products than the solvent candidates (**Appendix 2**).

However, in a comparison between biodegradation and ecotoxicity classification for 32 solvent candidates using EPI Suite™ and experimental results in marine biodegradation and ecotoxicity tests, the correlations between the EPI Suite™ and the experimental data were poor (Eide-Haugmo et al., 2012). SAR data should, therefore, be treated with great caution and should not be used as proof of any P or T properties for chemicals. However, it may be easier to use the SAR system for prediction of log Pow values of solvents and degradation products since these are related to poor water solubility and lipophilicity. Since all solvents and degradation products are water-soluble, possible B-properties of these substances are unlikely. No further actions were, therefore, taken for considering potential bioaccumulation factors of these substances.

Efforts to generate acute and chronic QSARs to conduct robust SSDs have been made for amine oxides, as they have shown to be highly toxic to aquatic organisms. These models are based on linear mathematical relationships, relying on octanol-water predicted partitioning coefficient of the compound log Kow and the measured effect concentrations to estimate the aquatic toxicity.

4.2 QSARs of amines

The aquatic toxicity of amine oxides (AO) was studied by Belanger et al. (2016) for generating toxicity QSARs at different chain lengths. They involved a fish (*Danio rerio*), an invertebrate (*Daphnia magna*) and an algae (*Desmodesmus subspicatus*) species. They also included an additional alga (*Ankistrodesmus falcatus*) and a macrophyte (*Lemna gibba*) specie to increase taxonomic diversity to generate a Species Sensitivity Distribution (SSD) for their AO aquatic toxicity studies. Algae appeared to be the most sensitive

group of aquatic organisms versus invertebrates and fish. The order of sensitivity from the most to the least one was algae > macrophyte > invertebrate > fish (Table 4.1). However, the sensitivity of each species was inversely related to the number of the amine chain length. The smaller the chain length, the higher the sensitivity.

The critical ecotoxicological endpoints for each test type were growth rate (acute and chronic interpretations) for algae, immobility or lethality for invertebrate and lethality for zebrafish. QSAR relationships for amine oxide toxicity to the aquatic species were developed using linear regression of the toxicity versus the chain length:

$$\log EC50 = (\log Kow) + \text{Chain length}$$

Table 4.1: Acute and chronic toxicity of amine oxides based on chain lengths to test species (Belanger et al., 2016).

Species	Chain length	Duration	Statistic	Toxicity value (mg l ⁻¹)	Effect
Algae					
<i>Desmodesmus subspicatus</i>	8	72h	EC50	126	Growth rate
<i>Desmodesmus subspicatus</i>	10	72h	EC50	4.93	Growth rate
<i>Desmodesmus subspicatus</i>	12	72h	EC50	0.467	Growth rate
<i>Desmodesmus subspicatus</i>	14	72h	EC50	0.0297	Growth rate
<i>Desmodesmus subspicatus</i>	16	72h	EC50	0.0133	Growth rate
<i>Desmodesmus subspicatus</i>	8	72h	EC10	42	Growth rate
<i>Desmodesmus subspicatus</i>	10	72h	EC10	2.02	Growth rate
<i>Desmodesmus subspicatus</i>	12	72h	EC10	0.105	Growth rate
<i>Desmodesmus subspicatus</i>	14	72h	EC10	0.0052	Growth rate
<i>Desmodesmus subspicatus</i>	16	72h	EC10	0.0064	Growth rate
<i>Ankistrodesmus falcatus</i>	12	7d	EC50	2.83	Growth rate
<i>Ankistrodesmus falcatus</i>	12	7d	EC10	0.767	Growth rate
Macrophyte					
<i>Lemna gibba</i>	12	7d	EC50	4.02	Growth rate
<i>Lemna gibba</i>	12	7d	EC10	0.240	Growth rate
Invertebrate					
<i>Daphnia magna</i>	8	48h	EC50	485.65	Immobilisation
<i>Daphnia magna</i>	10	48h	EC50	83.94	Immobilisation
<i>Daphnia magna</i>	12	48h	EC50	15.74	Immobilisation
<i>Daphnia magna</i>	14	48h	EC50	1.70	Immobilisation
<i>Daphnia magna</i>	16	48h	EC50	0.760	Immobilisation
Fish					
<i>Danio rerio</i>	8	96h	LC50	1237	Survival
<i>Danio rerio</i>	10	96h	LC50	743	Survival
<i>Danio rerio</i>	12	96h	LC50	26.2	Survival
<i>Danio rerio</i>	14	96h	LC50	2.48	Survival
<i>Danio rerio</i>	16	96h	LC50	0.26	Survival

Amine oxides' SSDs based on their chain length were generated with a 5th percentile hazardous concentration (HC5), ranging from 4.7 µg l⁻¹ to 52 µg l⁻¹. An assessment factor of 2 was applied as appropriate for PNEC generation due to the robustness of the SSD dataset. Thus, the resulting predicted no effect concentrations (PNEC) for amine oxides at different lengths were in the range of 2.35 µg l⁻¹ to 26 µg l⁻¹.

4.3 Ecotoxicity and biodegradation data of solvent candidates

4.3.1 Ecotoxicity data and PNECs

Data on acute ecotoxicity of the solvent candidates described in Table 3.1 were collected from various sources, including different review papers and reports, dossiers from the European Chemical Agency (ECHA) and experimental data of tests performed at SINTEF. Ecotoxicity tests performed at SINTEF were conducted according to 'Good Laboratory Practice' (GLP). Although this laboratory is not approved as a GLP laboratory for ecotoxicity testing at the time of writing this report, it has been previously approved, and the authors confirm that have maintained the same QA systems as during the GLP period. The information given in the ECHA dossiers are also important, since these dossiers mainly rely on GLP-studies, or otherwise describe the QA level of the tests.

Nearly all available data are from aquatic tests with freshwater or marine species. Most of the data were from acute tests, since very few chronic data were available. For consistency, have used acute data (EC50 or LC50) from tests with 'standard' organisms, representing the three trophic levels phytoplankton (algae), herbivores (copepods, crustaceans) and fish, and used these data for determination of PNEC concentrations of the solvent candidates. When several data are available from tests representing one trophic level, have used the lowest EC-50/LC-50 value, since it is assumed that this may represent the most sensitive species. A complete list with the ecotoxicity data is shown in **Appendix 3**, while Table 4.2 shows the data for each trophic level, with the results of the most sensitive species within each level, and the PNEC values determined from the most sensitive species within all three trophic levels. Although results from both freshwater and marine tests are represented, we have not differentiated between these. The data from the most sensitive species are used, irrespective of whether they are of marine or freshwater origin. There were not enough ecotoxicity data available in the literature to establish SSDs for any of the solvent candidates, which would result in lower assessment factors.

According to the results in Table 4.2, none of the solvent candidates should be considered to be 'Toxic' according to the PBT criteria (see Table 2.2 and Table 2.3). Although LOEC/NOEC data are given for only a few of the candidates (see **Appendix 3**), the most toxic candidates (piperidine and pyrrolidone) have EC50-values of 2-3 mg l⁻¹, which are factors of 200-300 higher the LOEC/NOEC threshold level of 0.01 mg l⁻¹.

Table 4.2: EC-50 or LC-50 results from ecotoxicity tests of the solvent candidates. Results are shown for three trophic levels, representing the most sensitive test species within each level. PNEC concentrations are determined from the toxicity data of the most sensitive species irrespective of trophic levels, using an assessment factor (AF) of 1,000.

Solvent	Phytoplankton	Invertebrates	Fish	PNEC (mg l ⁻¹)
	EC-50 (mg l ⁻¹)	EC-50 (mg l ⁻¹)	LC-50 (mg l ⁻¹)	
MEA	70	84	150	0.07
AP	21	500	10	0.01
AB	30	Not determined	Not determined	0.03
MIPA	39	109	220	0.04
DGA	493	>500	>681	0.49
MMEA	28	33	>100	0.07
EAE	27	35	147	0.03
DEA	357	100	540	0.10
DIPA	20	187	37	0.02
AEEA	920	>100	Not determined	0.01
BHE	582	Not determined	Not determined	0.58
DMMEA	40	112	110	0.04
MDEA	20	183	100	0.02
DEEA	23	67	Not determined	0.02
TEA	216	610	11800	0.22
DMPA	16	112	147	0.02
AMP	119	325	193	0.12
AMPD	158	316	>10,000	0.16
AEPD	78	668	460	0.08
TBEA	Not determined	Not determined	Not determined	Not determined
TBAB	35	17	Not determined	0.02
EDA	111	16	230	0.02
PDA	175	27	>100	0.03
DMPDA	483	Not determined	147	0.15
MAPA	56	76	Not determined	0.06
DETA	906	54	1,000	0.05
PETA	460	26	>220	0.03
Spermid	Not determined	Not determined	Not determined	Not determined
Spermin	Not determined	Not determined	Not determined	Not determined
ACHP	9	19	Not determined	0.009
DMAPA	34	60	122	0.03

Solvent	Phytoplankton	Invertebrates	Fish	PNEC
	EC-50 (mg l ⁻¹)	EC-50 (mg l ⁻¹)	LC-50 (mg l ⁻¹)	(mg l ⁻¹)
TMDPA	10	53	>100	0.01
TMBPA	8	50	21	0.008
PZ	316	10	52	0.01
EtOH-PZ	329	Not determined	6410	0.32
AE-PZ	674	69	Not determined	0.07
Morph	9	101	180	0.009
Piper	2	10	Not determined	0.002
2-Piper-EtOH	44	202	Not determined	0.044
EtOH-Piper	1,6	Not determined	>100	0,002
Pyrrrol	3	Not determined	Not determined	0.003
EtOH-Pyrrrol	15	143	Not determined	0.02
Ala	77	>10,000	Not determined	0.08
Sarc	>10,000	839	Not determined	0.84
Glyc	Not determined	Not determined	Not determined	Not determined
DMA	9	48	17	0.009
TeA	8	34	16	0.008
Sulfolane	500	171	>100	0.10

4.3.2 Biodegradation data and half-lives

Biodegradation data were collected from the same sources as the ecotoxicity data. Many biodegradability screening tests according to OECD Guidelines (Test methods 301 or 306) have been performed at SINTEF, and these were mainly supplemented with data from the ECHA dossiers. The predominant numbers of results are from aquatic tests, either from freshwater or seawater. The tests in freshwater and seawater may not be directly comparable if the freshwater tests are performed with activated sludge or sewage as microbial inocula. Since the seawater tests are performed with the seawater itself as inocula, the bacterial concentrations are higher in freshwater tests with sludge or sewage than in the seawater tests. Results from screening tests in freshwater with sludge or sewage have, therefore, often showed faster biodegradation than results from seawater tests, and these assumptions are recognised even by regulators (ECHA, 2017b; OECD, 2006). However, comparison of biodegradation screening tests performed at SINTEF with seawater and freshwater inocula did not show significant differences ($p > 0.05$; paired t-test) when the freshwater was not enriched with sludge or sewage, except DEEA and AMP which showed slower biodegradation in seawater than in freshwater (Figure 4.1).

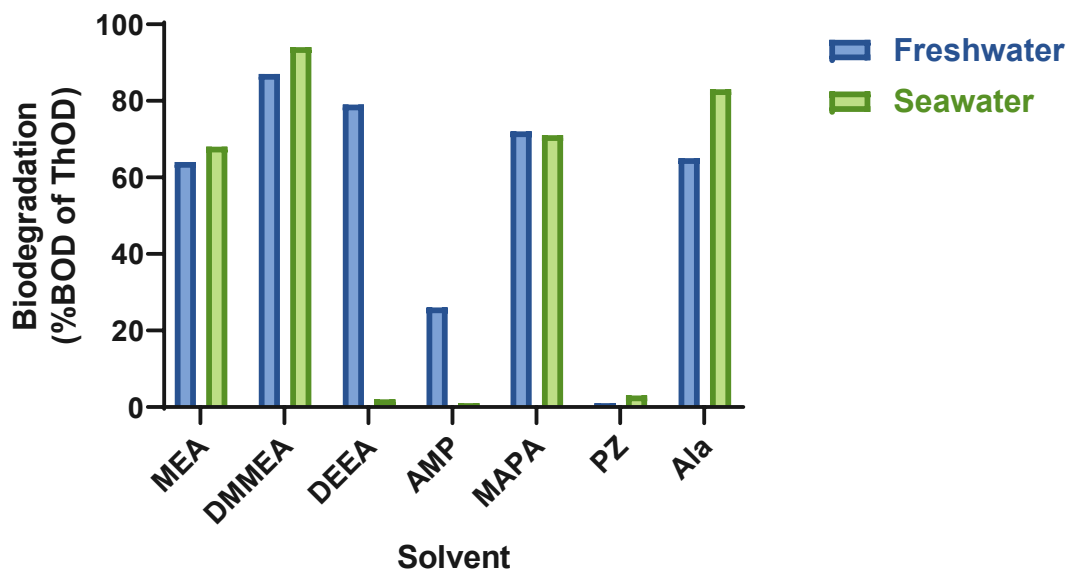


Figure 4.1: Ultimate biodegradation of solvents after 28 days of incubation in freshwater or seawater at 20°C. The results are percentage biochemical oxygen demand (BOD) of the theoretical oxygen demand (ThOD).

Ultimate biodegradation of the solvent candidates is shown in Table 4.3, separating between tests with high inoculum concentrations and tests performed with seawater or freshwater as single inoculum source. The latter tests have been performed SINTEF or at NTNU (Table 4.3 and **Appendix 3**). The results from the tests with high inoculum concentrations (sludge or sewage) are used to determine if the solvents are judged to be readily biodegradable if ultimate biodegradation was $\geq 60\%$, all retrieved from ECHA dossiers.

Some solvents lacked data from the ECHA dossiers, and only data from freshwater or seawater tests without inoculum enrichments were available. If biodegradation from these tests were $\geq 60\%$, these solvents are considered readily biodegradable. If biodegradation was $< 60\%$, we cannot exclude that the solvent is still readily biodegradable.

The half-lives determined for the solvent were used to determine if solvent candidates could be considered persistent (P) according to the PBT criteria (Table 2.2). The half-lives were determined as follows, based on the percentage ultimate biodegradation:

$$k = -\left(\frac{1}{\text{time}}\right) \times \ln\left(\frac{100 - \%BOD}{100}\right)$$

$$\text{Half - life (days)} = \frac{\ln 2}{k}$$


The k-values are in most instances determined from the % BOD after 28 days (time).

Table 4.3: Ultimate biodegradation results from screening tests of the solvent candidates. Results are shown as % ultimate biodegradation and half-lives in tests with enriched inoculum from sludge/sewage as described in ECHA dossiers, or % ultimate biodegradation and half-lives in freshwater (FW) or seawater (SW) not enriched (performed by SINTEF). Based on these data, the solvent candidates are judged as readily biodegradable and persistent. Where the results are based on more than one test, the range is given and the number of tests in brackets.

Solvent	Biodeg-ECHA dossiers		Biodeg-SINTEF/NTNU		Ready biodegradable	Persistent
	%	Half-life (d)	%	Half-life (d)		
MEA	62-83 (n=2)	11-20	78 (FW)	13 (FW)	Yes	No
AP	86	10	3 (SW)	>500 (SW)	Yes	No
AB	No data	No data	69 (SW)	17 (SW)	Yes	No
MIPA	60 (d3)	2	58 (SW)	22 (SW)	Yes	No
DGA	84	11	<1 (SW)	>500 (SW)	Yes	No
MMEA	93 (d21)	6	70 (SW)	17 (SW)	Yes	No
EAE	62	20	70 (SW)	16 (SW)	Yes	No
DEA	93	7	83 (FW)	11 (FW)	Yes	No
DIPA	94	7	<1 (SW)	>500 (SW)	Yes	No
AEEA	45	33	3 (SW)	>500 (SW)	No	No
BHE	No data	No data	30 (SW)	54 (SW)	Not determined	No
DMMEA	61 (d14)	8	87-94 (FW/SW)	7-9 (FW/SW)	Yes	No
MDEA	96 (d19)	4	77 (FW)	13 (FW)	Yes	No
DEEA	82 (d10)	4	<1-79 (FW/SW)	12.>500 (FW/SW)	Yes	No
TEA	No data	No data	20 (SW)	87 (SW)	Not determined	Not determined
DMPA	99	4	16 (SW)	111	Yes	No
1DMA2P	90	8	5 (FW)	378	Yes	No
AMP	89	9	83 (FW)	11 (FW)	Yes	No
AMPD	97 (d22)	4	4 (SW)	475	Yes	No
AEPD	6-8 (n=2)	233-246	4 (SW)	475	No	Not determined
TBEA	No data	No data	7	267	Not determined	Not determined
TBAB	43 (d42)	52	<1	>500	No	No
EDA	95	5	72 (SW)	15 (SW)	Yes	No
PDA	96 (d14)	5	72 (SW)	15 (SW)	Yes	No
DMPDA	No data	No data	6 (SW)	314 (SW)	Not determined	Not determined
MAPA	No data	No data	69-97 (n=4)	6-17	Yes	No
DETA	87 (d21)	7	3 (SW)	>500 (SW)	Yes	No
PETA	50	28	<1 (SW)	>500 (SW)	No	No
Spermid	No data	No data	100	4	Yes	No

Solvent	Biodeg-ECHA dossiers		Biodeg-SINTEF/NTNU		Ready biodegradable	Persistent
	%	Half-life (d)	%	Half-life (d)		
Spermin	No data	No data	88	9	Yes	No
ACHP	71	16	14	129	Yes	No
DMAPA	65 (d20)	13	55 (SW)	24 (SW)	Yes	No
TMDPA	10	184	30 (SW)	54 (SW)	No	No
TMBPA	60	21	72 (SW)	16 (SW)	Yes	No
PZ	39	39	<1-68 (FW/SW)	17->500 (FW/SW)	Yes	No
EtOH-PZ	No data	No data	<1 (SW)	>500	No	Not determined
AE-PZ	No data	No data	13 (FW)	139 (FW)	No	Not determined
Morph	91	8	22 (SW)	78 (SW)	Yes	No
Piper	67 (d14)	9	86 (SW)	10	Yes	No
2-Piper-EtOH	88	9	71 (FW)	16 (FW)	Yes	No
EtOH-Piper	52 (10d)	9	3 (FW)	>500 (FW)	Yes	Not determined
Pyrrol	95 (d9)	2	85 (SW)	10 (SW)	Yes	No
EtOH-Pyrrol	No data	No data	39 (FW)	39 (FW)	Yes	No
Ala	No data	No data	65-83 (n=2)	11-19	Yes	No
Sarc	No data	No data	72 (d15)-74	8-14	Yes	No
Glyc	No data	No data	68 (SW)	17 (SW)	Yes	No
DMA	88	9	77	13	Yes	No
TeA	No data	No data	35 (SW)	119 (SW)	Not determined	Not determined
Sulfolane	10 (d14)	92	3 (SW)	>500	No	Not determined

The data in Table 4.3 show that 36 of the 49 of the solvent candidates (69%) were judged to be both readily biodegradable and not persistent. Seven of the candidates were judged as not readily biodegradable, based on information in the ECHA dossiers. These included the secondary alkanolamine AEEA, the sterically hindered alkanolamines AEPD and TBAB, the secondary and tertiary polyamines PETA and TMDPA, the cyclic amine PZ, and the organic-sulphuric compound Sulfolane. However, in a test performed at NTNU, PZ was readily biodegradable by 67% after 28 days (Henry et al., 2017). In addition, ready biodegradability was questionable for 7 candidates lacking data from ECHA dossiers, and with <60% biodegradation in tests performed at SINTEF. These included the secondary and tertiary alkanolamines BHE and TEA, the sterically hindered alkanolamine TBEA, the primary polyamine DMPDA, the cyclic amines EtOH-PZ and AE-PZ, and the volatile amine TeA. Since the tests performed at SINTEF and NTNU have used water as inoculum, these seven solvent candidates may still be readily biodegradable when tested with sludge or sewage as inoculum. Sewage and sludge contain higher bacterial concentrations

	Document	Deliverable D3.1
	Issue date	03 Feb 2023
	Dissemination level	Public

than water used in the SINTEF tests, and studies have shown that bacterial concentrations are important for degradation rates (Martin et al., 2018).

While the tests described in Table 4.3 are a mixture of freshwater and marine tests, it is also relevant to mention that biodegradation may be faster in freshwater than marine tests. Henry et al. (2017) presented the biodegradability of selected amines tested used for CO₂ capture under aerobic and anoxic conditions. MEA showed the fastest biodegradability of all tested amines, followed by DEA; while AMP, MDEA and PZ were degraded approximately after one week, under aerobic conditions (Table 4.4). AMP and MDEA showed half-lives of approximately 14 days compared to more than 700 days under marine conditions, while DEA and MEA had also shorter apparent half-lives in freshwater than in sea water. These results showed improved biodegradability compared to seawater, especially for AMP and MDEA which have been reported persistent and undegraded under marine conditions (Brakstad et al., 2012; Eide-Haugmo et al., 2012). In general, the microbial associations played a major role in the biodegradability of amines.

Table 4.4: Comparison of half-lives (in days) and ultimate biodegradation between fresh and sea water (Henry et al., 2017).

Amine	t ^{1/2} Half-life (d)		BOD (% of ThOD)	
	Fresh water	Sea water ^a	Fresh water	Sea water ^{a,b}
AMP	12.5	>700	83.3	<1 ^b
MEA	8.4	8.3	78.5	71.2 ^a ; 68 ^b
DEA	9.2	24.1	83.2	66.3a; 62.8 ^b
MDEA	13.5	>700	77.3	<1 ^{a,b}
PZ	17.1	-	67.9	3.0 ^b

^a Brakstad et al., 2012; ^b Eide-Haugmo et al., 2012

Based on the data provided in Table 4.3, none of the solvent candidates can be judged as persistent, since testing beyond screening is required. Of the seven candidates judged as not readily biodegradable, only two can be judged as questionable with respect to persistence (AEPD and Sulfolane). However, six of the seven candidates with questionable ready biodegradability properties were also questionable with respect to persistence, including TEA, TBEA, DMPDA, EtOH-PZ, AE-PZ and TeA. Further investigations of the nine candidates with questionable persistence were conducted:

- AEPD: An inherent biodegradation test with activated sludge resulted in >90 % biodegradation after seven days, according to the ECHA dossier for this substance. Although the substance is not readily biodegradable, it can be considered to be *not persistent*. These data are further strengthened by SAR data with estimated ultimate time factor of 3.0682 (**Appendix 2**), which is higher than the time factor of 2.25-2.75 for potential P or vP substances.

- Sulfolane: Shake-flask studies with soil or sediment as inocula showed complete degradation of sulfolane at 8°C after 27 days and after 13 days at 28°C (Greene et al., 2000, 1998). Sulfolane can, therefore, be considered as *not persistent*. This was further supported by SAR data with estimated ultimate time factor of 3.6744 (**Appendix 2**).
- TEA: Studies in surface soils showed 90 % primary biodegradation after 2 weeks (Kookana et al., 2022). A biodegradation experiment in sediment-water described in the ECHA dossier further resulted in ultimate biodegradation half-lives of 7 days. TEA can, therefore, be considered to be *not persistent*. This was further supported by SAR data with estimated ultimate time factor of 3.7328 (**Appendix 2**).
- TBEA: No further data were found and the *persistence of this substance remains questionable*. SAR data predicted the substance to be not persistent, with an estimated ultimate time factor of 3.6979 (**Appendix 2**).
- DMPDA: According to the ECHA dossier DMPDA showed 5 % inherent biodegradation after 28 days, proving that the substance was not inherently biodegradable. No further data were found and the persistence of this substance remains questionable. SAR data predicted the substance to be not persistent, with an estimated ultimate time factor of 3.6334 (**Appendix 2**).
- EtOH-PZ: No further data were found and the *persistence of this substance remains questionable*. SAR data predicted the substance to be not persistent, with an estimated ultimate time factor of 3.5446 (**Appendix 2**).
- AE-PZ: According to the ECHA dossier, a test performed according to OECD301F with a substrate concentration of 30 mg l⁻¹ showed little or no biodegradation, and the substance was shown to be toxic or inhibitory to the activated sludge inoculum at this concentration. No further data were found and the *persistence of this substance remains questionable*. SAR data were also questionable, with an estimated ultimate time factor of 2.7077 (**Appendix 2**).
- TeA: A bacterial strain isolated from a wastewater treatment pool with TeA was able to biodegrade 100 mg l⁻¹ TaA to ammonia in 32 hours (Cai et al., 2011). TeA (55 mg l⁻¹) was also shown to be removed by mixed acclimated cultures in a wastewater treatment system by stream with a half-life of approximately 10-75 hours (Wang et al., 2007). There are several further reports on culture systems removing TeA rapidly from wastewater, since this substance is an odorant which is preferably removed from these systems. However, no reports on biodegradation with non-acclimated water or cultures have been found. However, according to the ECHA dossier this substance is considered readily biodegradable based on decisions by the European regulator. It is, therefore, concluded that TeA is *not persistent*. SAR data are inconclusive, since an estimated ultimate time factor of 2.7207 is described for the substance (**Appendix 2**).

4.4 Ecotoxicity and biodegradation data of potential degradation products

Several potential degradation products of solvent amines have been identified, either as minor components in the solvent mixtures, after thermal or oxidative degradation in the facilities, or after emissions to the environment. Some of these products have been identified during previous projects, like the TCM Amine project (Brakstad et al., 2010), or during MEA and CESAR1 campaigns (Languille et al., 2021; Morken et al., 2017a; Moser et al., 2020). However, most attention has been paid to the potential formation of the carcinogenic nitrosamines and nitramines. Stable nitrosamines can form from secondary

and tertiary amine solvents (Masuda et al., 2000; Nielsen et al., 2012; Reynolds et al., 2012), while nitramines can form from both primary, secondary or tertiary amines (Sørensen et al., 2015). While nitrosamines are rapidly degraded photolytically, nitramines are photolytically stable (Sørensen et al., 2015). Nitrosamines and nitramines may be found as minor constituents in solvents and emitted to the air (Morken et al., 2017a).

The potential degradation products considered in this study are described in Table 3.2.

4.4.1 Ecotoxicity data and PNECs

In the same manner as with the solvent candidates (Table 3.1), data on acute ecotoxicity of the degradation products from solvent candidates were collected from various sources, including different review papers and reports, dossiers from the European Chemical Agency (ECHA) and experimental data of tests performed at SINTEF. In addition, the EPA ECOTOX database has been consulted for provision of some data (<https://cfpub.epa.gov/ecotox/>), mainly on nitrosamines and nitramines, which are not registered in the REACH Substance factsheets. Ecotoxicity and biodegradation data for 58 degradation product candidates of eleven substance groups were assessed. A complete list with the ecotoxicity data is shown in **Appendix 4**, while Table 4.5 shows the data for each trophic level, with the results of the most sensitive species within each level, and the PNEC values determined from the most sensitive species within all three trophic levels. As observed from the **Appendix 4** and Table 4.5, ecotoxicity data lacked for several products, and in those cases, we have used SAR data for PNEC determination (see **Appendix 2**).

Table 4.5: EC50 or LC50 results from ecotoxicity tests of the potential degradation products. Results are shown for three trophic levels (where available), representing the most sensitive test species within each level. PNEC concentrations are determined from the toxicity data of the most sensitive species irrespective of trophic levels, using an assessment factor (AF) of 1,000. When 'reliable' data are not available, PNECs are determined from SAR data (see Appendix 2).

Solvent	Phytoplankton	Invertebrates	Fish	PNEC (mg l ⁻¹)
	EC-50 (mg l ⁻¹)	EC-50 (mg l ⁻¹)	LC-50 (mg l ⁻¹)	
Acetic acid	301	426	293	0.3
Oxalic acid	19	162	160	0.02
Bicine	4,930	>100	124	0.12
HEPD	No data	527	195	0.20
HeGly	No data	No data	No data	No data ^b
Ammonia ^a	13,000	137	43	0.04
Formaldehyde	4.2	29	24	0.004
Acetaldehyde	36	48	31	0.03
Ethylene glycol	3,199	>100	>72,850	0.10
Acetone	530	2,100	5,540	0.53
Acetonitrile	400	400	730	0.40
Methylamine	47	163	970	0.05

Solvent	Phytoplankton	Invertebrates	Fish	PNEC
	EC-50 (mg l ⁻¹)	EC-50 (mg l ⁻¹)	LC-50 (mg l ⁻¹)	(mg l ⁻¹)
Dimethylamine	9	50	918	0.009
Ethylamine	1,6	7.8	118	0.002
Diethylamine	34	58	27	0.03
Ethyl-methylamine	17	309	No data	0.02
Propylamine	No data	71	46	0.05
2-Methyl-2-(methylamino)propane-1-ol	No data	No data	No data	No data ^b
Nitromethane	3.01	103	455	0.003
Nitroethane	17	22	596	0.02
HEED	46	>100	No data	0.05
Formamide	125	>500	6,562	0.13
Acetamide	>10,000	>10,000	No data	10
HEF	No data	No data	No data	0.30 ^c
HEA	100	100	No data	0.10
HEHEAA	No data	No data	No data	No data ^b
BHEOX	No data	No data	No data	No data ^b
Piperazine	316	10	52	0.01
HEPO	No data	No data	No data	No data ^c
Morpholine	9	101	180	0.009
4-Acetomorpholine	No data	580	6,812	0.58
Imidazole	No data	342	284	0.28
HEI	30	No data	No data	0.03
HEIA	1,057	>100	1,004	0.01
Pyrrrole	No data	No data	No data	0.03 ^d
1,1'-(1,3-Phenylene)bis-1H-pyrrole-2,5-dione	67	2.06	0.188	0.0002
Pyrazine	No data	No data	No data	0.74 ^c
Methylpyrazine	No data	No data	No data	0.36 ^c
Dimethylpyrazine	No data	No data	No data	0.18 ^c
Oxazolidine	>10,000	No data	No data	10
4,4-Dimethyloxazolidine	>10,000	No data	No data	10
NDELA	No data	No data	No data	0.3 ^c
NPIP	No data	No data	No data	No data ^b
NDEA	No data	230	775	0.23

Solvent	Phytoplankton EC-50 (mg l ⁻¹)	Invertebrates EC-50 (mg l ⁻¹)	Fish LC-50 (mg l ⁻¹)	PNEC (mg l ⁻¹)
NDMA	No data	300	200	0.20
NMEA	No data	No data	No data	0.04 ^c
NMOR	84	No data	No data	0.08
NDPA	No data	No data	5.9	0.006
NPYR	No data	No data	No data	0.03 ^c
NPZ	No data	No data	No data	0.04 ^c
DNPZ	No data	No data	170	0.17
NO-HeGly	No data	No data	No data	No data ^b
DMNA	>2,000	3,042	No data	2.0
MEA-NO ₂	2,535	>2,500	No data	2.5
MNA	754	1,426	No data	0.75
PZ-NO ₂	430	1,031	No data	0.43
AMP-NO ₂	871	1,094	No data	0.87
DENA	No data	No data	No data	No data ^b

^a Results for ammonium chloride used; ^b No test or SAR information available; ^c Based on SAR information; ^d LOEC

The results shown in Table 4.5 showed that PNECs were determined for all except for three degradation products, where no test or SAR information was found. These substances included 2-methyl-2-(methylamino)propane-1-ol, the nitrosamine nitropiperidine, and the nitramine diethylnitramine. If these products are detected in CC emissions, ecotoxicity tests would be of importance to execute. In addition, test information was lacking for a number of substances, which included N-(2-hydroxyethyl)formamide (HEF), pyrrole, pyrazine, methylpyrazine, dimethylpyrazine, N-nitrosodiethanolamine (NDELA), nitroso-N-methylethylamine (NMEA), nitrosopyrrolidine (NPYR) and nitrosopiperazine (NPZ). Since only SAR data were used for PNEC determinations, these data are of limited reliability and should be supplemented with test data, if some of these substances occur in emissions.

4.4.2 Biodegradation data and half-lives

Biodegradation data were mainly collected from the same sources as the ecotoxicity data. In addition, SINTEF has performed different types of biodegradation tests during different projects, including screening tests for determination of ultimate biodegradation and studies of primary biodegradation with low substrate concentrations in simulation tests with non-amended water as bacterial sources. Ultimate biodegradation data from screening tests are summarised in Table 4.6 and shown in more detail in **Appendix 5**. Only organic compounds are subject to biodegradation, and ammonia was, therefore, not included in this data set.

For twelve of the 58 potential degradation products tested, no ultimate biodegradation data were identified (Table 4.6), and these should be subject to testing if detected in emissions. Twenty of the


degradation products with available screening data could be considered readily biodegradable, while 22 were not readily biodegradable. As previously described, these are not possible to judge with respect to potential persistence from tests for ready biodegradability. For several of the degradation products there are no available data, or inadequate data have been reported from emission campaigns, including oxazolidinone, N-(2-hydroxyethyl)imidazolidinone (HEIA) and N-(2-Hydroxyethyl)ethylenediamine (HEED) from MEA campaigns (Moser et al., 2020).

Table 4.6: Ultimate biodegradation results from screening tests of potential degradation products. Results are presented as % biodegradation, with day of measurement in brackets if this is not the standard 28 days. The half-lives were calculated from the biodegradation results. Results from ECHA dossiers were mainly determined in tests with enriched inoculum from sludge/sewage. When reliable data were not available, biodegradation data were also searched from other sources, including tests performed at SINTEF. Based on the data, the solvent candidates are judged as readily biodegradable and persistent, if appropriate.

Solvent	Biodeg-ECHA dossiers		Data other		Readily biodegradable ^a	Persistent ^a
	%	Half-life (d)	%	Half-life (d)		
Acetic acid	No data	2.0	No data	No data	Yes	No
Oxalic acid	89 (d5)	1.6	No data	No data	Yes	No
Bicine	77 (d14)	6.6	No data	No data	Yes	No
HEPD	15	119	No data	No data	No	Nd
HeGly	No data	No data	No data	No data	No data	No data
Formaldehyde	91 (d14)	4.0	No data	No data	Yes	No
Acetaldehyde	80 (d14)	6.0	No data	No data	Yes	No
Ethylene glycol	83 (d14)	5.5	No data	No data	Yes	No
Acetone	76 (d20)	9.7	No data	No data	Yes	No
Acetonitrile	No data	No data	30 (d14)	27	Nd	Nd
Methylamine	96	6.0	No data	No data	Yes	No
Dimethylamine	96	6.0	77	13	Yes	No
Ethylamine	90	8.4	No data	No data	Yes	No
Diethylamine	69	17	No data	No data	Yes	No
Ethyl-methylamine	67	18	No data	No data	Yes	No
Propylamine	78	13	No data	No data	Yes	No
2-Methyl-2-(methylamino)propane-1-ol	No data	No data	No data	No data	No data	No data
Nitromethane	10	184	No data	No data	No	Nd
Nitroethane	1	>500	No data	No data	Yes	No
HEED	No data	No data	1	>500	Nd	Nd
Formamide	60	21	No data	No data	Yes	No
Acetamide	69 (d11)	6.5	No data	No data	Yes	No

Solvent	Biodeg-ECHA dossiers		Data other		Readily biodegradable ^a	Persistent ^a
	%	Half-life (d)	%	Half-life (d)		
HEF	No data	No data	No data	No data	No data	No data
HEA	48	30	No data	No data	No	Nd
HEHEAA	No data	No data	No data	No data	No data	No data
BHEOX	No data	No data	No data	No data	No data	No data
Piperazine	39	39	No data	No data	No	No
HEPO	No data	No data	No data	No data	No data	No data
Morpholine	91	8	22	78	Yes	No
4-Acetomorpholine	60	21	No data	No data	Yes	No
Imidazole	90	8.4	No data	No data	Yes	No
HEI	No data	No data	No data	No data	No data	No data
HEIA	1	>500	No data	No data	No	Nd
Pyrrrole	95 (d9)	2.1	85	10	Yes	No
1,1'-(1,3-Phenylene)bis-1H-pyrrole-2,5-dione	1	>500	No data	No data	No	Nd
Pyrazine	No data	No data	No data	No data	No data	No data
Methylpyrazine	No data	No data	No data	No data	No data	No data
Dimethylpyrazine	22	78	No data	No data	No	Nd
Oxazolidine	No data	No data	No data	No data	No data	No data
4,4-Dimethyloxazolidine	No data	No data	No data	No data	No data	No data
NDELA	No data	No data	17	104	No	Nd
NPIP	No data	No data	1	>500	No	Nd
NDEA	No data	No data	1	>500	No	Nd
NDMA	No data	No data	1	>500	No	Nd
NMEA	No data	No data	1	>500	No	Nd
NMOR	No data	No data	1	>500	No	Nd
NDPA	No data	No data	1	>500	No	Nd
NPYR	No data	No data	1	>500	No	Nd
NPZ	No data	No data	1	>500	No	Nd
DNPZ	No data	No data	1	>500	No	Nd
DMNA	No data	No data	3.5	>500	No	Nd
MEA-NO ₂	No data	No data	33	49	No	No
MNA	No data	No data	34	47	No	No
PZ-NO ₂	No data	No data	3	>500	No	Nd
AMP-NO ₂	No data	No data	20	87	No	Nd
DENA	No data	No data	No data	No data	No data	No data

^a Nd, not determined

	Document	Deliverable D3.1
	Issue date	03 Feb 2023
	Dissemination level	Public

4.4.3 Ammonia and eutrophication

One degradation product, ammonia, was not included in Table 4.6 since it is not an organic compound. However, microbial oxidation of ammonia and ammonium salts may result in nitrite/nitrate formation (nitrification), and these nitrogen compounds are well known as fertilizers and may add to the local environmental nitrogen budgets. Elevated concentrations of ammonia may, therefore, result in eutrophication and may impact sensitive ecosystems and/or contribute to soil acidification on a local scale.

4.5 Nitrosamines and nitramines

Nitrosamines and nitramines are of particular concern as degradation products in CC facilities, due to their carcinogenic properties. Degradation products, including nitrosamines and nitramines, will form in CC plants from reactions between the amine solvent and NO_x species in the flue gas. For primary amine solvents (e.g., MEA), nitrosamines can only be formed indirectly from other degradation products. Solvents with secondary and tertiary amine functionalities (e.g., piperazine and *n*-methyldiethanolamine) can form stable nitrosamines. Nitramines can form directly from primary, secondary, or tertiary amines (da Silva et al., 2013). No data on environmental properties of nitrosamines and nitramines were available from the ECHA dossiers since these are produced commercially in very low quantities.

4.5.1 Ecotoxicity

The ecotoxicity summary in Table 4.5 indicated PNEC-values for nitrosamines of 0.006 (NDPA) to 0.17 (DNPZ) mg l⁻¹ and 0.43 (PZ-NO₂)-2.5 (MEA-NO₂) mg l⁻¹ for nitramines. However, the PNEC estimations are only based on a limited number of acute tests. A few chronic studies of nitrosamine effects have been performed, as summarised by Brooks (2008). Chronic values ranged from 0.025 – 200 mg l⁻¹ for growth inhibition of a marine algae (*Tetraselmis maculata*), with a LOEC value of 0.025 mg l⁻¹ after seven days exposure (AUBERT, 1982; Brooks, 2008). Chronic effects to rainbow trout (*Oncorhynchus mykiss*) exposed to NDMA for 1 year (52 weeks) showed an increase in the presence of hepatocellular carcinomas at the lowest exposure concentration of 200 mg kg⁻¹ (Brooks, 2008; da Silva et al., 2012; Grieco et al., 1978).

Acute and chronic endpoints of the two nitramines DMNA and MEA-NO₂ are shown in Table 4.7 for marine algal, copepod and fish species (the phytoplankton *Skeletonema costatum*, the oyster *Crassostrea gigas*, and the juvenile turbot *Scophthalmus maximus*). DMA-NO₂ was found to be the more toxic of the two compounds, with the most sensitive LOEC found in algae and oyster embryos, even at moderate concentrations. In contrast, MEA-NO₂ showed a significant effect on the oyster larvae development only at a concentration of 100 mg l⁻¹. No significant mortality was observed for the rest of the species (Coutris et al., 2015). The calculated PNECs of their studies were 0.08 mg l⁻¹ for DMNA and 0.18 mg l⁻¹ for MEA-NO₂, which were lower than the PNECs determined from the acute tests shown in Table 4.5. Further studies may, therefore, be required for improving the ecotoxicity data needed for PNEC determinations of these substances.

As shown in Table 2.2, a substance should have a NOEC or LC10 < 0.01 mg l⁻¹ for marine or freshwater organisms to be classified as Toxic according to the PBT-criteria. Based on these data, the nitrosamines and nitramines do not represent products associated with Toxicity according to these criteria.

In case of the genotoxicity assessment, MEA-NO₂ that was found to have a higher potency than DMA-NO₂ by three orders of magnitude. Significantly elevated levels of DNA damage (84%) were observed at the lowest MEA-NO₂ concentration tested (1 mg l⁻¹) and as concentration increased to > 3 mg l⁻¹, there was no DNA left. On the other hand, in case of DMA-NO₂, a concentration of up to 100 mg l⁻¹ was required to cause 37% DNA damage (Coutris et al., 2015).

Table 4.7: Ecotoxicity parameters for marine species exposed to A) DMA-NO₂ and B) MEA-NO₂; NOEC: No-Observed Effect Concentration; LOEC: Lowest Observed Effect Concentration; ECx: concentration giving a x% effect.

Species effect	NOEC (mg l ⁻¹)	LOEC (mg l ⁻¹)	EC ₁₀ (mg l ⁻¹)	EC ₅₀ (mg l ⁻¹)
A) DMA-NO₂				
Oyster larval development 24h	21	45	39	47
Copepod mortality 48h	≥100	>100	na	na
Turbot mortality 96h	≥100	>100	na	na
Algal growth 72h	18	32	48	591
Macroalgae growth 14d	<100	100	na	na
Copepod reproduction 14d	25	50	8	70
Turbot growth 28d	≥100	>100	na	na
B) MEA-NO₂				
Oyster larval development 24h	45	100	65	107
Copepod mortality 48h	≥100	>100	na	na
Turbot mortality 96h	≥100	>100	na	na
Algal growth 72h	>100	>100	na	na
Macroalgae growth 14d	100	500	na	na
Copepod reproduction 14d	50	100	18	108
Turbot growth 28d	≥100	>100	na	na

4.5.2 Biodegradation

According to the data of ultimate biodegradation, most of the tested nitrosamines and nitramines were poorly biodegradable in screening tests and are therefore candidates for possible Persistence according to the PBT criteria, with half-lives >60 in seawater and >40 days in freshwater/estuarine water (Table 2.2). Primary biodegradation studies of nitrosamines and nitramines have been performed with low substrate concentrations as CSIRO (Williams et al., 2011) and at SINTEF (Brakstad et al., 2018), and the results are summarised in Table 4.8. These data showed that the nitrosamines NDELA, NDMA and NMEA were not persistent according to the PBT criteria, while particularly the cyclic nitrosamines (NPIP, NMOR, NPYR, NPZ, DNPZ) are still suspected candidates for persistency, according to these studies. However, the cyclic nitrosamines NPIP and NPYR were depleted in soil column with constant flow-through of lake water, simulating a groundwater system, with half-lives of 4-7 days determined by pseudo first-order rates (Drewes et al., 2006). The depletion was faster in columns with well adapted than in columns with non-

adapted microbial communities, emphasising the need for adapted communities for efficient dissipation of nitrosamines (Bradley et al., 2005; Drewes et al., 2006).

The nitramines MEA-NO₂ and AMP-NO₂ were also subject to primary biodegradation at low concentrations, while the other nitramines are still candidates for persistency.

Table 4.8: Primary biodegradation of nitrosamines and nitramines at low concentrations in aquatic systems. The results are summaries of two experimental studies performed at CSIRO using activated wastewater (Williams et al., 2011) or in normal water collected from a lake and a river (Brakstad et al., 2018). Biodegradation was performed at 20-22°C and is shown as % degradation with incubation time in brackets, and as half-lives, based on first-order rate determinations.

Substrate	CSIRO		SINTEF	
	Biodegradation (%) ^a	Half-life (days)	Biodegradation (%) ^a	Half-life (days)
NDELA	Not analysed		24	32
NPIP	<10	Not determined	<10	>500
NDEA	~ 25	Not determined	<10	>500
NDMA	~ 10 (d5)	1.2	<10	>500
NMEA	~ 20	9.2	<10	>500
NMOR	<10	No determined	<10	>500
NDPA	<10	Not determined	<10	>500
NPYR	<10	Not determined	<10	>500
NPZ	Not analysed		<10	>500
DNPZ	<10	Not determined	<10	>500
DMNA	Not analysed		<10	>500
MEA-NO ₂	Not analysed		27	28
MNA	Not analysed		<10	>500
PZ-NO ₂	Not analysed		<10	>500
AMP-NO ₂	Not analysed		27	35
DENA	Not analysed		<10	>500

^a biodegradation after 28 days of incubation, if not other days are described in brackets

In these studies, concentrations in ranges of 1-200 µg l⁻¹ were used, and comparison of different concentrations (10 µg l⁻¹ and 100 µg l⁻¹) showed that biodegradation was faster at the lower concentration (Williams et al., 2011). This was confirmed in studies with 14C-labelled NDMA in lake water, where the nitrosamine in eight different concentrations (162 ng l⁻¹ to 15 mg l⁻¹) were tested (Kaplan and Kaplan, 1985). Comparison of different incubation temperatures (20°C, 10°C and 5°C) showed temperature-dependences, with Q₁₀-values for NDELA of 1.5, MEA-NO₂ of 2.3 and AMP-NO₂ of 3.9. An aquatic survey between different water types lakes showed that parameters such as lower pH, lower concentrations of NH₄⁺, NO₃⁻ and total P could explain the lower degradation rate (Brakstad et al., 2018).

The nitrosamines and nitramines which were biodegradable in the SINTEF study were all alkanol-compounds, and biodegradation of these will result in formation of alkyl-compounds (Figure 4.2).

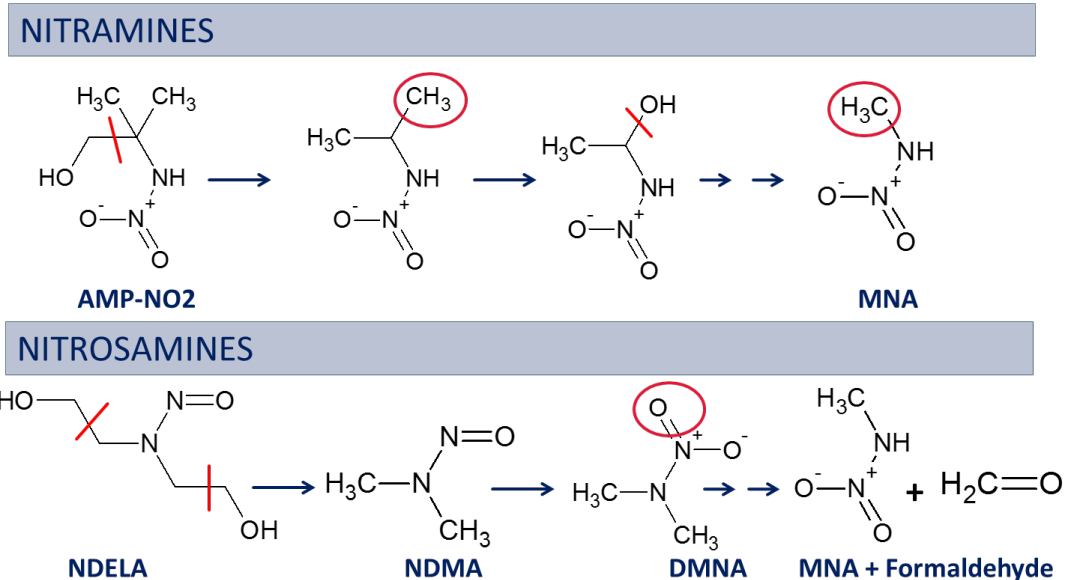


Figure 4.2: Expected biodegradation pathways of nitramines and nitrosamines, as shown for AMP-NO₂ and NDELA (sources Pathway Prediction System" of the University of Minnesota Biocatalysis-Biodegradation Database (UM-BBD); Fournier et al., 2006).

A study performed at SINTEF comparing target-specific primary biodegradation of NDELA and total nitrosamine (TONO) analyses showed that while primary biodegradation was fast, total nitrosamines remained in the water (Figure 4.3). This confirmed the model data described in Figure 4.3, that alkanolnitrosamines may be biodegraded to alkyl nitrosamines. Further degradation of alkyl nitrosamines will result in the formation of alkylamines or nitramines by microbes harbouring monooxygenases, while bacteria with dioxygenases are not able to degrade nitrosamines (Sharp et al., 2007, 2005).

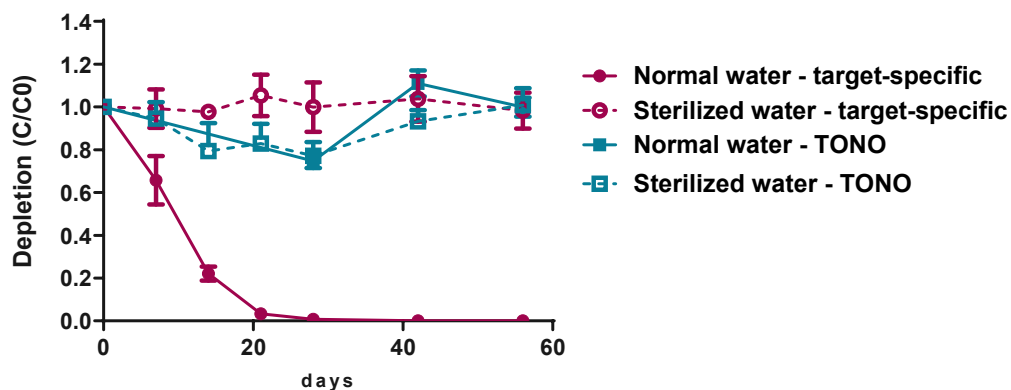


Figure 4.3: Target-specific depletion of NDELA (LC-MS analyses) and total nitrosamine (TONO) in normal and sterilised lake water (Source: SINTEF).

4.5.3 Other degradation mechanisms

Other degradation processes than biodegradation will include hydrolysis and photolysis. It is generally assumed that nitrosamines and nitramines are not susceptible to hydrolysis, but other structural properties might influence this resistance. Different studies have found nitrosamines and nitramines to be hydrolytically stable for >1 year under both laboratory (Sørensen et al., 2015) and natural conditions (Williams et al., 2011). Hydrolysis studies of five nitrosamines (NDELA, NPZ, NDMA, NMOR and DNPZ) and four nitramines (DMNA, MEA-NO₂, PZ-NO₂ and MNA) at pH 4, 7 and 9 at 50°C, revealed that nitrosamines and nitramines were generally resistant to hydrolytic degradation in the pH-range 4–9 (Sørensen et al., 2015). However, the nitrosamine and nitramine derivatives of piperazine (NPz and Pz-NO₂), although they were hydrolytically stable at pH 4 and pH 9, a ~30% degradation was observed at pH 7 and 50 °C. In addition, in a CSIRO study, the nitrosamines were found to be stable to hydrolysis after five days even at a high temperature (50°C) in pH 4, 7 and 9. This elevated temperature, was assumed to be equivalent to hydrolytic stability over a 1-year period at 25°C (Williams et al., 2011).

While nitramines were not susceptible to photolytic degradation, nitrosamines were photolytically degraded with absorption peaks at ~230 nm and ~330 nm wavelengths (Sørensen et al., 2015). Experimental and theoretically photolytic decay half-lives of the degradable nitrosamines are shown in Table 4.9 (Sørensen et al., 2015).

Table 4.9: Experimental and theoretically determined half-lives of the nitrosamines NDMA, NDELA, NMOR and NPZ (Sørensen et al., 2015). Experimental half-lives represent average sunlight conditions at 50° latitude. Estimated half-life values are presented for both summer and winter conditions and based on quantum yields (Φ) of both 1 (maximum estimated half-life; OECD 316) and 0.5 (expected experimental half-life (Plumlee and Reinhard, 2007)).

Nitrosamine	Experimental half-life (minutes)		Estimated half-life (minutes)		
	60 W m ⁻²	Summer ($\Phi=1$)	Summer ($\Phi=0.5$)	Winter ($\Phi=1$)	Winter ($\Phi=0.5$)
NDMA	7.5±0.5	15	30	92	184
NDELA	6.4±0.1	10	20	61	122
NMOR	6.1±0.2	17	34	111	222
NPZ	10.6±0.6	15	30	90	180

The half-lives of the nitrosamines were estimated to be less than 20 min under summer conditions and less than two hours under winter conditions, as shown in Table 4.9. These values are relevant for the surface layers of natural freshwaters receiving standard sunlight levels (Sørensen et al., 2015). These results were confirmed by studies performed at CSIRO (Williams et al., 2011). In the CSIRO studies, photolytic degradation rates of nitrosamines ranged from 11 -24 minutes by simulation of midday summer solar irradiation at the latitude of Mongstad (Norway) in clean water. Even during winter at Mongstad, where theoretical midday insolation levels were up to 13 times less than those found in summer, there is sufficient irradiance for nitrosamines to have half-lives of hours. The slowest rate of photolysis determined for the nitrosamines was still more than 400 times faster than the biodegradation case (Williams et al., 2011). Other studies have also confirmed fast photolytic degradation in water. In a study of aqueous photolysis of seven alkyl nitrosamines (NDMA, NMEA, NDEA, NDPA, NDBA, NPyr and

NPip) by irradiation in a solar simulator (direct photolysis at irradiances of 765 W m^{-2} , representing Southern California midsummer, midday sun) half-lives of all nitrosamines were less than 25 minutes in water, as shown in Table 4.10 (Plumlee and Reinhard, 2007).

As shown in Figure 4.4, the proposed photolytic degradation of a nitrosamines were performed by preferential attack of the nitroso-group, resulting in the transformation of NDELA to MEA (Sørensen et al., 2015). Alkanolnitrosamines, therefore, rapidly lose their nitrosamine properties as a result of photolysis, in contrast to the biodegradation process, where alkanolamines are biodegraded to alkylamines by preferential attack of the hydroxyl-groups (Figure 4.2).

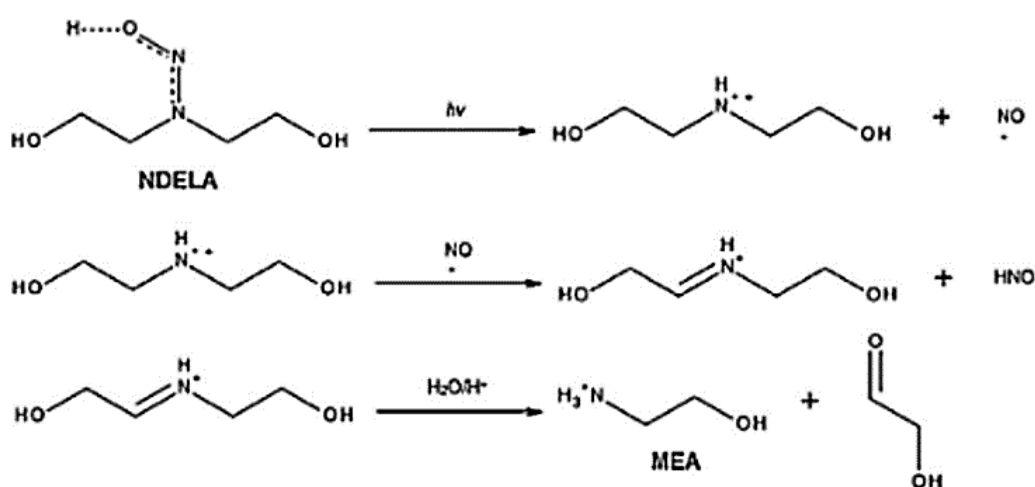


Figure 4.4: Proposed photolytic degradation products of NDELA by cleavage of the nitroso group (Sørensen et al., 2015).

Table 4.10: Direct photolysis rate and quantum yields for tested nitrosamines (Plumlee and Reinhard, 2007).

Amine	$T_{1/2}$ Half-life (min) ¹	$t^{1/2}$ Half-life (min) ²	Quantum yield (Φ) ³	Quantum yield (Φ) ⁴
DNPZ	-	11.1	0.41	0.38
NDMA	16	21.7	0.41	0.32
NMEA	15	22.7	0.61	0.63
NDEA	15	24	0.43	0.31
NDPA	14	22	0.46	0.21
NDBA	15	-	0.52	-
NMOR	17 (summer) ⁵ ; 111 (winter) ⁵	16	-	0.23
Npyr	14	22.7	0.55	0.31
NPip	12	18.4	0.51	0.76

¹ Plumlee and Reinhard, 2007: Irradiation 765 W/m^2 ; initial concentrations were $100 \mu\text{g l}^{-1}$; except NPip at $1000 \mu\text{g l}^{-1}$

² CSIRO, 2011: Irradiation 520 W/m^2 ; initial concentrations were $10 \mu\text{g l}^{-1}$ over a 60-min exposure

³ Plumlee and Reinhard, 2007: The quantum yield (Φ) of a photochemical reaction describes the moles of reactant transformed per moles of photons absorbed; that is the averaged value over the wavelength range at which the nitrosamine absorbs sunlight

⁴ CSIRO, 2011: The quantum yield (Φ)

⁵ Sørensen et al., 2013: 50° latitude

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The UV-vis absorption spectra for NDMA and the other nitrosamines, from different studies (Lee et al., 2005; Plumlee and Reinhard, 2007; Sørensen et al., 2013) showed two absorption bands with maxima near 230 and 330 nm. The nitrosamine absorption band near 230 nm was below the range of natural sunlight, but the less intense band at 330–340 nm overlaps is within the wavelength range corresponding to solar irradiation at the earth's surface, being responsible for the photodecay of nitrosamines in the environment. The absorption peak of nitrosamines at 330–340 nm may be explained by the $n \rightarrow \pi^*$ transition by electron excitation from an oxygen lone-pair to an anti-bonding π orbital in the $-N=O$ group (Sørensen et al., 2015). Nitrosamine quantum yields are 10–100 times larger than that of some other photosensitive environmental contaminants.


Nitramines are potentially released in much smaller quantities than the nitrosamines to surface or ground waters. However, since they will neither photodegrade nor hydrolyse, they may be quite persistent in these environments (if not biodegraded) and may be more of a concern. Nitramines do not have the chromophoric and unsaturated $-N=O$ group, but rather a $-NO_2$ group which makes the $n \rightarrow \pi^*$ impossible. A number of other environmental factors, such as concentration and type of natural organic material and the amount of particulate material present in surface waters will have a significant impact on the level of nitrosamine.

4.5.3.1 Effect of pH

Photolysis of nitrosamines has shown to be pH dependent, with the rate of photolytic loss being generally faster under acidic conditions with alkaline conditions not being favourable for photolysis. For example, Lee et al. 2005 reported that high NDMA concentration and acidic conditions favour the formation of dimethylamine, and note that at NDMA concentrations expected in wastewater, methylamine is the major expected amino product with only trace amounts of dimethylamine generated. Aqeel et al. (2017) also investigated the effect of pH UV photodegradation of NDELA), NDEA and NMOR. They showed that photodegradation of the nitrosamines was possible over the entire pH range (2–10) investigated, but was quite rapid in acidic conditions, resulting in half-lives less than 10 min. To understand the photodegradation pathways of the nitrosamines, the behaviour of the degradation products was also investigated. MEA with DEA, EA with DEAE and MOR were confirmed as the main amino products of NDELA, NDEA, and NMOR respectively. An increase in the concentration of parent secondary amines (DEA, DEAE and MOR) was observed in basic (pH10) to weakly acidic conditions (pH 4) during photodegradation of the nitrosamines. In contrast, a decrease in the concentration of primary amines (MEA and EA) was observed in basic (pH10) to weakly acidic conditions (pH 4) (Aqeel et al., 2017). Lee et al. (2005) found that the NO_2^- concentration was highly correlated with dimethylamine formation during NDMA photodegradation.

4.5.3.2 Effect of Natural Organic Matter (NOM)

Irradiation experiments performed in surface water showed that the presence of DOM did not enhance nitrosamine photolysis via an indirect sensitization, as has been observed for some other organic contaminants. In fact, the rapid nitrosamine decay tended to be slower in the presence of DOM, indicative of light screening (Plumlee and Reinhard, 2007). Sørensen et al. (2015) investigated the effect of light screening by NOM on NDELA as a representative compound. They showed a linear relationship between increasing NOM concentration in the water and the $t_{1/2}$ of NDELA. Increasing the NOM concentration from

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1 mg l⁻¹ to 100 mg l⁻¹ gave a three-fold increase in the $t_{1/2}$ of NDELA. Both Plumlee and Reinhard (2007) and Sørensen et al. (2015) indicated that nitrosamine $t_{1/2}$ will be significantly influenced by the concentration of NOM present in surface waters, with high NOM concentrations leading to longer residence times.

As environmental concentrations of nitrosamines are predicted to be low in the range 1–10 ng l⁻¹, NOM might outcompete nitrosamines for photons, effectively reducing their degradation rate. Degradation rates were significantly hindered at a NOM concentration of 10 mg l⁻¹ and become negligible at a NOM concentration of 100 mg l⁻¹ NOM (under summer conditions). This indicated that environmentally relevant concentrations of nitrosamines may persist in natural waters, especially where the NOM concentration is quite high (Sørensen et al., 2015). However, it is important to consider that the waters will constantly be replenished with more nitrosamine from emissions. As a result, the final environmental concentration will depend upon the balance between decay and nitrosamine emissions.

It is important to note that although nitrosamines seem to degrade rapidly by photolysis under natural sunlight, this degradation is dependent on the presence of sunlight. As a result, the release of nitrosamines at night or in parts of the world where there are long periods of the year with no daylight can significantly decrease the importance of this degradation pathway.

5 The CEASAR1 solvent

5.1 Physical-chemical and environmental data of solvent amines

The SCOPE project has a specific focus on the CESAR1 solvent, which is a mixture of AMP and piperazine (Figure 5.1), with a relative distribution of 3 M AMP and 1.5 M piperazine. Some physical-chemical properties of the solvent amines relevant for environmental risk assessments are shown in Table 5.1, while data relevant for the fate in the environment are shown in Table 5.2.

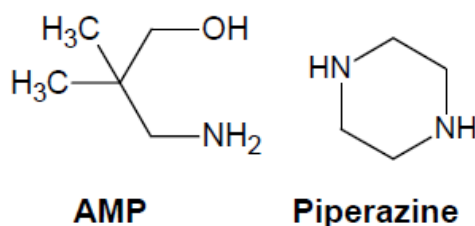


Figure 5.1: Chemical structures of AMP and piperazine.

Table 5.1: Physical-chemical data for AMP and piperazine (Brakstad et al., 2010).

Abbreviation	AMP	Piperazine
SMILES	CC(N)CO	C1CNCCN1
CAS	124-68-5	110-85-0
Molecular weight (g mol ⁻¹)	89.14	86.14
Physical state	Solid	Solid
Colour	Clear	White - yellow
Odour	Amine	Ammonia
pH	9-10,5	12
Vapour pressure	1.33 hPa	15mbar
Viscosity (mPa)	102	
Boiling point (°C)	165	146 - 148
Freezing/melting point (°C)	31-32	107 - 111
Autoignition temperature (°C)	438	320
Flash Point (°C)	67	65
Explosion limit lower (vol %)		4
Explosion limit higher (vol %)		14
Solubility in water (mg l ⁻¹)	1,000,000	150,000
Specific gravity/density	0.934	
Molecular weight (g mol ⁻¹)	89.1	86.14
Log Pow	-1.19	-1.5
Solubility in oil	7.927 × 10 ⁻⁴	

Table 5.2: Hazard and fate data of AMP and piperazine. Hazard and biodegradation data originate from tests performed at SINTEF, while data for Henry's Law constant, bioaccumulation/bioconcentration and soil adsorption are collected from EPI Suite™ SAR data. Hydrolysis data are based on tests performed in the CESAR project (Brakstad et al., 2010).

Hazard/fate data	AMP	Piperazine
Acute toxicity phytoplankton – EC50 (mg l ⁻¹)	119	316
Acute toxicity invertebrates – EC50 (mg l ⁻¹)	325	10
Acute toxicity fish – LC50 (mg l ⁻¹)	193	52
PNEC (mg/L)	0.119	0.010
Henry's Law constant (Pa m ⁻³ mol)	6.57 × 10 ⁻⁵	9.42 × 10 ⁻⁶
Octanol-water coefficient (logPow)	-0.74	-0.80
Bioconcentration factor	0.91	1.56
Soil adsorption partition coefficient (logKoc)	0.404	1.313
Photodegradation half-lives (days)	0.4	0.06
Hydrolysis (%)	Not significant	Not significant
Primary biodegradation 20°C rate coefficient (k)	0.077	0.125
Primary biodegradation 20°C half-life (days)	9.0	5.5
Primary biodegradation 10°C rate coefficient (k)	0.077	0.028
Primary biodegradation 10°C half-life (days)	9.0	24.6
Primary biodegradation 5°C rate coefficient (k)	0.022	0.0045
Primary biodegradation 5°C half-life (days)	32	153
Ultimate biodegradation 20°C rate coefficient (k)	10.6 × 10 ⁻³	1.088 × 10 ⁻³
Ultimate biodegradation 20°C half-life (days)	65	>500

5.2 Solvent ecotoxicity

The ecotoxicity of the CESAR1 solvent was performed in the CESAR project and reported in the deliverable 1.3.3 of the project (O.G Brakstad et al., 2010). The ecotoxicity data of the solvent and solvent amines are shown with the freshwater phytoplankton species *P. subcapitata* and the invertebrate *Daphnia* sp. In Table 5.3.

The results of Table 5.3 showed that the EC50 of AMP and piperazine varied relatively little between the different solvents, from 711 to 1,271 mg l⁻¹ for the algae and 69 to 325 mg l⁻¹ for the invertebrate. The data show that the acute solvent toxicities are moderate or low for the amines. The solvent CESAR1 also showed comparable EC50 values for the two species (201 and 421 mg l⁻¹). Despite the fact that both AMP

and piperazine were slightly more toxic to the invertebrate than the algae, the CESAR1 solvent displayed higher EC50 values (less toxic) in the invertebrate than the algal assay.

Table 5.3: Acute toxicity of AMP, piperazine and CESAR1 solvent to the algal freshwater species *P. subcapitata* and the invertebrate *Daphnia sp.* The results are shown as the concentrations inhibiting algal growth or causing invertebrate immobilisation for 50% (EC50) of the populations. The results are shown as average results with 95% confidence intervals (C.I.) of replicates.

Amine/solvent	Species	EC50 (lower – higher 95% C.I.) mg l ⁻¹
AMP ^{A)}	<i>P. subcapitata</i>	711 (633-799)
	<i>Daphnia sp.</i>	325 (259 – 406)
Piperazine ^a	<i>P. subcapitata</i>	1,271 (1,241-1,303)
	<i>Daphnia sp.</i>	69 (59– 80)
CESAR1 ^b	<i>P. subcapitata</i>	201 (192 – 209)
	<i>Daphnia sp.</i>	421 (208-854)

^a Pure amines; ^b CESAR1 as solvent in a water solution with 3M AMP and 1.5M piperazine

Based on the acute toxicities of AMP and piperazine, the additive toxicities of the solvent amines were determined and calculated for a mixture of 3M AMP and 1.5 M piperazine, using the method described by French-McCay (French-McCay, 2002). If the toxicities of these amines in mixture were additive, the calculated and experimentally measured toxicities of the CESAR1 should be comparable for the two species. Calculated and experimental toxicities against *P. subcapitata* and *Daphnia sp.* are shown in Figure 5.2.

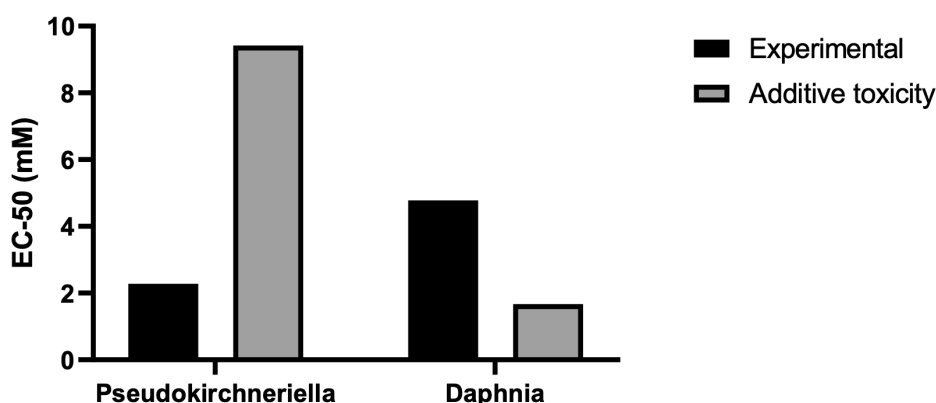


Figure 5.2: Acute toxicity of the CESAR1 solvent to the algal species *P. subcapitata* and the invertebrate *Daphnia sp.* The results are shown as EC-50 determines experimentally and by calculations of additive toxicity.

The results of Figure 5.2 showed some deviations between experimental data and additive toxicity calculations. While additive toxicity data resulted in lower toxicity than experimental data with the algae *P. subcapitata*, the opposite was the result with the invertebrate *Daphnia* sp. Explanations for the differences between the experimental and calculated data could include lack of purities in the amine mixtures, and possible deviations between nominal and actual amine concentrations in the solvent mixture

Since these results were based only on single testing, further testing of the amines and different binary mixtures of these amines were performed with the marine zooplankton *Calanus finmarchicus* (Hansen et al., unpublished). The 96 h-LC50 for AMP and piperazine were determined using standard ecotoxicity testing for this species and calculated at 159 (146.8-172.2) mg l⁻¹ and 147.3 (138.4-156.9) mg l⁻¹ for AMP and piperazine, respectively. Binary mixtures were prepared keeping concentrations of AMP constant and piperazine varying and vice versa to assess mixture toxicity. When AMP concentration was constant at 79.5 mg/L, and piperazine concentration added to reach 96 h-LC50 for the mixture was 78.55 (70.99-86.9) mg l⁻¹ piperazine. Vice versa, when PIZ was kept constant at 73.7 mg l⁻¹, the AMP concentration added to reach 96 h-LC50 for the mixture was 78.08 (63.55-95.94) mg l⁻¹.

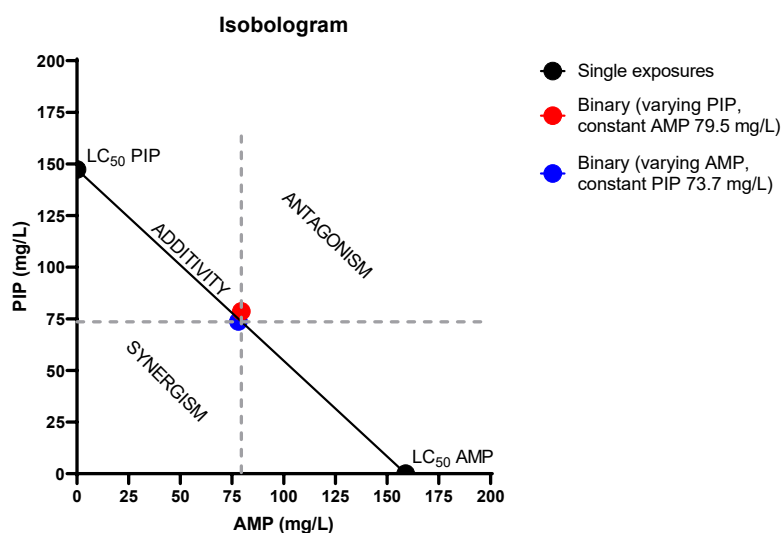


Figure 5.3: Isobologram for acute toxicity data for AMP and PIZ singly and in mixtures.

An isobologram (Figure 5.3), where the concentration of piperazine was plotted as a function of AMP concentration. The LC50 for both amines were plotted on the x-axis and y-axis for AMP and piperazine, respectively, and a line is drawn between them. If the LC50 for the mixtures are on this line, additive toxicity is shown. If the plotted data are above to the right of the line, the binary mixture displays antagonistic effects, whereas if the plotted data are below, there are synergistic effects between the two amines. As observed in Figure 5.3, both binary mixture tests showed that these two amines display additive toxicity (Hansen et al., unpublished). These results also emphasise the need for more elaborate data than single tests for evaluation of additive toxicity.

6 Assessing potential impacts of emissions

6.1 Relative contribution of components to environmental risk

Although hazard environment is only environmentally relevant for emissions reaching aquatic and terrestrial soil environments, emissions from the source can also be monitored to determine the potential distributions of hazardous components. The relative distributions of components of environmental concern may thereby be identified and emissions mitigated by response actions to remove or reduce components of concern from the emissions. Environmental monitoring is for instance well established in the offshore industry to reduce discharges of potential hazardous components from produced water discharges.

Based on information of relative component distributions from two MEA and one CESAR1 campaign at TCM, such a hazard distribution monitoring was conducted. The two MEA campaigns were performed in 2014 and 2015 (Morken et al., 2017, 2014), while the CESAR1 campaign was performed in 2019-2020 (Languille et al., 2021). The toxicity distributions were determined from the PNEC values described in Table 4.2 and Table 4.5. The toxicity distributions are shown in Table 6.1, Table 6.2 and Table 6.3, and the illustrated in Figure 6.1.

Table 6.1: Relative toxicity distribution, PNEC of total emission and PEC/PNEC of the emissions from a MEA campaign at TCM in 2014 (Morken et al., 2014).

Compound	Conc. (ppmV)	Conc (µM)	PNEC (µM)	Toxicity contribution (fraction/PNEC × 10 ⁻⁴)	Toxicity contribution (%)
MEA	8.9	0.37	1.15	4.1	0.083
NH ₃ (ammonium chloride)	18,266	755.11	2.35	4,079.0	83.129
Methylamine	2.5	0.10	1.61	0.8	0.017
Formaldehyde	43	1.78	0.10	231.5	4.717
Acetaldehyde	455	18.81	0.68	350.4	7.142
Acetone	88	3.64	9.13	5.1	0.103
Acetic acid	12	0.50	5.00	1.3	0.026
Formamide (FA)	13	0.54	2.89	2.4	0.048
Acetamide	14	0.58	114.78	0.1	0.001
Nitromethane	20	0.83	0.05	213.4	4.350
Nitroethane	0.8	0.03	0.27	1.6	0.032
Pyrrrole*	5	0.21	0.45	5.9	0.120
Pyrazine	107	4.42	9.24	6.1	0.124
Pyrazinemethyl	23	0.95	3.83	3.2	0.064
Pyrazinedimethyl	7	0.29	1.66	2.2	0.045
SUM	18,610.2	788.14		4,906.9	100
PNEC-Mix (µM)				2.04	
PEC/PNEC				386.73	

Table 6.2: Relative toxicity distribution, PNEC of total emission and PEC/PNEC of the emissions from a MEA campaign at TCM in 2015 (Morken et al., 2017).

Compound	Conc. (ppmV)	Conc (µM)	PNEC (µM)	Toxicity contribution (fraction × 10 ⁻⁴)	Toxicity contribution (%)
MEA	7	0.29	1.1460	3.93	0.09
NH ₃	15,500	640.76	2.3488	4,242	97.5
Dimethylamine	26.5	1.10	0.1996	85.3	1.96
Ethylamine	0.7	0.03	0.0444	9.42	0.22
Methylamine	23.5	0.97	1.6103	9.38	0.22
Diethylamine	0.01	0.00	0.4102	0.02	0.0004
Ethyl-methylamine	0.2	0.01	0.3384	0.28	0.007
Propylamine	0.1	0.00	0.8459	0.08	0.002
SUM	15,558	643.2		4,350	100
PNEC-Mix (µM)				2.30	
PEC/PNEC				280	

Table 6.3: Relative toxicity distribution, PNEC of total emission and PEC/PNEC of the emissions from an CESAR1 campaign at TCM in 2019-2020 (Languille et al., 2021).

Compound	Conc. (ppmV)	Conc (µM)	PNEC (µM)	Toxicity contribution (fraction × 10 ⁻⁴)	Toxicity contribution (%)
AMP	377	4.23	1.35	2,227	12.5
Piperazine	0.4	0.005	0.12	28.4	0.16
Formaldehyde	48	1.60	0.13	8,507	47.8
Acetonitrile	46	1.12	9.74	81.5	0.46
Acetaldehyde	50	1.14	0.68	1,182	6.6
Acetone	300	5.17	9.13	401	2.3
Ethylamine (MMA)	13	0.29	0.04	4,608	25.9
Formamide (FA)	6	0.13	2.89	32.7	0.18
Morpholine (Morph)	8	0.09	0.10	630	3.5
4,4-Dimethyloxazolidine (DMO)	5	0.05	98.86	0.4	0.002
2-Methyl-2-(methylamino)propane-1-ol (MeAMP) ^a	2.5	0.01	0.62	14.8	0.083
4-acetylmorpholine (AMOR)	3	0.02	4.49	3.7	0.021
2-Pentyl-1H-imidazol (C8H14N2) ^b	35	0.25	2.03	88.6	0.50
SUM	893.9	14.1		17,805	100
PNEC-Mix (µM)				0.56	
PEC/PNEC				25	

^a PNEC data for AMP used; ^b Tentative identification; PNEC data for imidazole used.

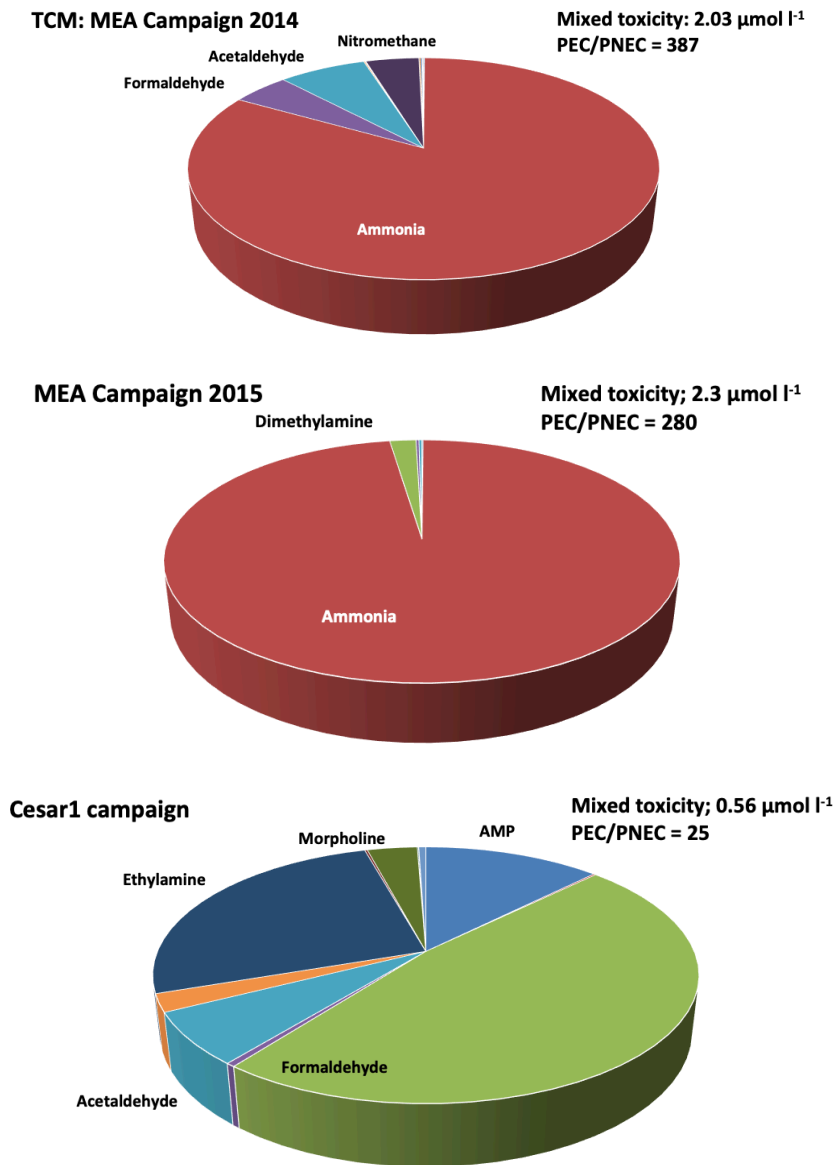



Figure 6.1: Relative toxicity distributions of compounds in TCM MEA and CESAR1 emission campaigns. The distributions show the relative PNEC contributions of emission compounds in relation to concentrations. The distributions were determined to estimate total PNECs of the emissions and the PEC/PNECs, based on the total concentrations of emission compounds measured.

In Table 6.1 – Table 6.3, the volumetric concentrations given and the PNECs were calculated to molar concentrations, using the gas constant for calculations from volumetric units (ppmV). The toxicity contributions were determined by the additive toxicity equation (French-McCay, 2002), and the toxicity contributions determined. From these calculations, the total PNECs of the emissions could be estimated and compared to the calculated concentrations (PEC). By comparing the PEC and PNEC values, it is possible to determine the dilutions required in the air before PEC-values become lower than the PNEC

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(Figure 6.1). The highest contribution to the toxicity from the MEA campaigns was ammonia. PNEC data were not used for ammonia itself, but for ammonium chloride since ammonia is expected to occur as ammonium ions in the environment at neutral pH. Although ammonium has low acute toxicity, the high emission concentrations resulted in its predominant contribution to the PNEC of the emission. In addition, ammonia and ammonium may locally contribute to eutrophication processes. In the CESAR1 campaign there was no information about ammonia in the emissions, and the toxicity contributions were therefore predominated by other products, like formaldehyde, ethylamine and AMP. The calculated PEC was lower from the CESAR1 than the MEA campaigns, and the PEC/PNEC lower, although the PNEC itself was lower for the CESAR1 than the MEA campaigns (Figure 6.1). It must be emphasised that these calculations are highly dependent on the chemical monitoring of the emissions since compounds not analysed for will not be included in the budget.

6.2 Potential environmental impact of discharge scenarios

A study to assess the environmental impact of amine emissions based on a worst-case scenario to derive maximum tolerable emissions of amines from CO₂ capture at Technology Centre Mongstad (TCM) was established by Karl et al. (2011). The operating conditions were reflected with typical and elevated emissions, a low MEA scenario with emissions of 40 tonnes yr⁻¹ MEA and 5 tonnes yr⁻¹ diethylamine (DEAE), and a high MEA scenario, with emissions of 80 tonnes yr⁻¹ MEA and 15 tonnes yr⁻¹ DEAE.

Maximum tolerable emissions of MEA and DEAE were defined as the highest emissions of these amines from the CO₂ capture facility that are tolerable with respect to safety limits in deposition. These *maximum tolerable emissions* of the solvent amines (Table 6.4 and Table 6.5) were determined dividing the emission rate by the exceedance factor of the emission source strength; that is the maximum model output concentration of the compound in wet deposition divided by the critical (safety) concentration level. That means that an increase of the MEA emission rate will result in a higher maximum concentration of MEA.

Based on the maximum deposition flux calculated, the critical annual deposition rate of 14.2 mg m⁻² for MEA, corresponding to a safety limit with respect to aquatic organisms of 7.5 µg l⁻¹, would be exceeded by a factor of 3 and 7, based on the low and high scenario, respectively. Similar, the maximum annual wet deposition flux of nitrosamines for DEAE would exceed the critical annual deposition rate of 0.047 mg m⁻² for the aquatic organisms by a factor of 4 and 11 in the low and high scenarios.


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Table 6.4: Summary of maximum tolerable emission results for methylamine (MEA) from the worst-case scenario (Karl et al., 2011).

Compound	Safety limit (ng l ⁻¹)	Critical deposition flux (mg m ⁻²)	Deposition flux max (mg m ⁻²)		Exceedance		Max. Tolerable MEA emission (tonnes yr ⁻¹)	Target/receptor
			MEA-LOW	MEA-HIGH	MEA-LOW	MEA-HIGH		
MEA	7,500	14.2	46	92	3.2	6.5	12	Aquatic algae
Nitramines	200	0.38	0.46	0.92	1.22	2.43	33	Aquatic fish
Formamide	24,000	45.4	23	46	0.51	1.01	79	Aquatic invertebrate

Table 6.5: Summary of maximum tolerable emission results for diethylamine (DEAE) from the worst-case scenario (Karl et al., 2011).

Compound	Safety limit (ng l ⁻¹)	Critical deposition flux (mg m ⁻²)	Deposition flux max (mg m ⁻²)		Exceedance		Max. Tolerable DEAE emission (tonnes yr ⁻¹)	Target/receptor
			MEA-LOW	MEA-HIGH	MEA-LOW	MEA-HIGH		
DEAE	200,000							Aquatic algae
Nitrosamines	25	0.047	0.17	0.52	3.6	10.9	1.4	Aquatic algae
Nitramines	200	0.38	1.84	5.52	4.9	14.6	1.0	Aquatic fish

The lowest maximum tolerable MEA emission in the aquatic environment was found to be 12 tonnes yr⁻¹; while, in case of DEAE, the lowest maximum tolerable emission was defined by the hazard of nitrosamines to drinking water, that is 0.4 tonnes yr⁻¹. The MEA-low and MEA-high scenarios for DEAE (5 and 15 tonnes yr⁻¹, respectively) were 5 and 15 times above the max tolerable DEAE emissions for the aquatic environment. Therefore, maximum wet deposition flux of nitrosamines and nitramines exceeded the safety limit for the aquatic environment when MEA and DEAE emissions are greater than 12 and 5 tonnes yr⁻¹, respectively.

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7 Conclusions

- According to PBT criteria, most solvent chemicals (amines), including MEA and PZ, can be considered readily biodegradable, non-bioaccumulative and non-toxic.
- Primary and secondary amino and hydroxyl groups are more degradable than tertiary amines and compounds containing quaternary carbon.
- Due to limited ecotoxicity data, especially chronic data, PNECs for amines are derived using large assessment factors (typically 1,000). More data would warrant SSD estimations, potentially reducing PNECs significantly.
- Based on available acute PNEC values, derived from SAR data, acute ecotoxicity for degradation products is higher than for the solvents; and although, none of the solvent candidates are considered to be toxic, the EC50 values for piperidine and pyrrolidine are 200-300 higher than the threshold level.
- Additivity may be used to explain mixture toxicity of amines in binary mixtures, but more complex emissions need to monitor and take into account contribution from degradation products.
- The Whole Effluent Toxicity together with the PBT assessment are recommended as tier-based approach for the RBA of produced waters.
- In aquatic systems, nitrosamines, while resistant to hydrolysis in water at various pH, degrade rapidly by photolysis under natural sunlight although the degradation rate can be significantly impacted by normal environmental concentrations of NOM. Degradation will decrease with increasing depth in the water column and be limited when nitrosamines are rapidly transported to environmental compartments where there is little or no light penetration (e.g., deeper waters and groundwater).
- Attention should be paid at the environmental fate of nitrosamines during winter periods (low temperatures and short days); The half-lives of nitrosamines are estimated to be higher in such conditions, as compared to summer.
- Photolysis is a particularly important pathway for the degradation of nitrosamines; pH effect on the UV photolysis of different N-nitrosamines shows strong photolabilities in acidic solution, while increasing DOC concentration leads to a decrease in the photodecay rate of nitrosamines. Nitramines, on the other hand, do not degrade by photolysis.
- Nitrosamines are susceptible to photolytic degradation at two absorption bands, with peaks at 230 and 330 nm wavelengths.
- Although nitramines exhibit resistance towards photodegradation, they are formed in sufficiently low quantities and disperse quickly enough that they will most likely reach environmental concentrations significantly below limits and they will be less of concern from a toxicological perspective.

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- Biodegradation of nitrosamines is shown to be temperature-dependent; with increased biodegradation at higher temperatures; however, it also differs between different nitrosamines. In addition to temperature-dependency, concentration levels and water type seem to play an important role, with biodegradation being faster at lower concentrations and under freshwater conditions.
- Most of the tested nitrosamines and nitramines are reported to be poorly biodegradable and are candidates for persistency.
- Previous ecotoxicity tests on freshwater phytoplankton and invertebrate species for the CESAR1 solvent (a mixture of AMP and piperazine which is the main focus solvent in the SCOPE project) have shown a higher EC50 (i.e. it less toxic) for invertebrates than phytoplankton.
- According to US EPA ECOTOX database, nitrosamines are relatively more acutely toxic to phytoplankton than to invertebrates and fish. Both experimental and SAR data indicated that the ecotoxicities of both compound groups were in the order algae > herbivores (Daphnia) > fish.

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Appendix 1: Predicted environmental concentrations determined according to the Technical Guidance Document.

A1.1 Atmospheric compartment

Table A1.1: Elements, input data and calculated output to PEC_{local} for the air compartment.

Elements	Input data	Output calculations	Term
Release (tonnes y ⁻¹)	X		RELEASE
Local direct emission (kg d ⁻¹)		X	E _{local,air}
Fraction of release at local source (-)	X		F _{mainsource}
Days of emission (d y ⁻¹)	X		T _{emission}
Local indirect emission to air (kg d ⁻¹)		X	E _{stp,air}
Fraction of emission to air from STP (-)	X		F _{stp,air}
Local concentration in air during emission (mg m ⁻³)		X	C _{local,air}
Annual average concentration in air 100 m from point source (mg m ⁻³)		X	C _{local,air,ann}
Annual average predicted environmental concentration in air (mg m ⁻³)		X	PEC _{local,ann}
Regional concentration in air (mg m ⁻³)	X		PEC _{air, regional}
Vapour pressure of substance (Pa)	X		V _p
Fraction of substance associated with aerosol particles (-)		X	F _{ass,aer}
Henry's Law constant (Pa m ⁻³ mol ⁻¹)	X		Log HENRY
Total deposition flux during emission episode (mg m ⁻² d ⁻¹)		X	DEP _{total}
Annual average total deposition flux (mg m ⁻² d ⁻¹)		X	DEP _{total,ann}

$E_{local,air}$ (kg d⁻¹) = Local direct emission rate to air during episode:

$$E_{local,air} = F_{mainsource} \times \frac{1000}{T_{emission}} \times RELEASE_{air} \quad (1)$$

$RELEASE_{air}$ = Release during life cycle stage to the air (tonnes yr⁻¹) – Input data

$F_{mainsource}$ = Fraction of release at the local main source at life cycle stage (-) – Input data

$T_{emission}$ = Number of days per year for the emission at life cycle stage (d yr⁻¹) – Input data

$E_{stp,air}$ (kg d⁻¹) = Local indirect emission to air from STP during episode:

$$E_{stp,air} = F_{stp,air} \times E_{local,water} \quad (2)$$

$F_{stp,air}$ = Fraction of the emission to air from STP (-) – Input data

$E_{local,water}$ = Local direct emission rate to water during episode (kg d⁻¹) – eq (1) for water compartment

$C_{std,air}$ = Concentration in air at source strength of 1 kg d⁻¹ (mg m⁻³) – 2.78×10^{-4}

$C_{local,air}$ = Local concentration in air during emission episode (mg m^{-3})

$$C_{local,air} = \max (E_{local,air} \times Estp_{air}) \times Cstd_{air} \quad (3)$$

$C_{local,air,ann}$ = Annual average concentration in air, 100 m from point source (mg m^{-3})

$$C_{local,air,ann} = C_{local,air} \times \frac{T_{emission}}{365} \quad (4)$$

$PEC_{local,air,ann}$ = Annual average predicted environmental concentration in air (mg m^{-3}):

$$PEC_{local,air,ann} = C_{local,air,ann} + PEC_{regional,air} \quad (5)$$

$PEC_{regional,air}$ = regional concentration in air (mg m^{-3}) – input data

$F_{ass,aer}$ = Fraction of the substance associated with aerosol particles (-)

$$F_{ass,aer} = \frac{CONjunge \times SURF_{aer}}{VP + CONjunge \times SURF_{aer}} \quad (6)$$

$CONjunge$ = constant of Junge equation (Pa m^{-1})

$SURF_{aer}$ = surface area of aerosol particles ($\text{m}^2 \text{m}^{-3}$) – Default: $CONjunge \times SURF_{aer} = 10^{-4} \text{ Pa}$

VP = Vapour pressure (Pa) – Input data

DEP_{total} = Total deposition flux during emission episode ($\text{mg m}^{-2} \text{d}^{-1}$):

$$DEP_{total} = (E_{local,air} + Estp_{air}) \times (F_{ass,aer} \times DEP_{std,aer} + (1 - F_{ass,aer}) \times DEP_{std,gas}) \quad (7)$$

$DEP_{std,aer}$ = Standard deposition flux of aerosol-bound compounds at a source strength of 1 kg d^{-1} ($\text{mg m}^{-2} \text{d}^{-1}$) – default value 1×10^{-2}

$DEP_{std,gas}$ = Deposition flux of gaseous compounds as a function of Henry's Law constant at a source strength of 1 kg d^{-1} ($\text{mg m}^{-2} \text{d}^{-1}$)

$$\text{Log HENRY} \leq -2: 5 \times 10^{-4}$$

$$\text{Log HENRY} -2 \text{ to } 2: 4 \times 10^{-4}$$

$$\text{Log HENRY} \geq 2: 3 \times 10^{-4}$$

Log Henry = \log_{10} of Henry's Law constant ($\text{Pa m}^{-3} \text{mol}^{-1}$) – Input data for each substance

$DEP_{total,ann}$ = Annual average total deposition flux ($\text{mg m}^{-2} \text{d}^{-1}$):

$$DEP_{total,ann} = DEP_{total} \times \frac{T_{emission}}{365} \quad (8)$$

A1.2 Soil compartment

Table A1.2: Elements, input data and calculated output to PEClocal for the soil compartment.

Elements	Input data	Output calculations	Term
Henry's Law constant (Pa m ⁻³ mol ⁻¹)	X		Log HENRY
Air-water partition coefficient (-)		X	K _{air-water}
Partition coefficient organic carbon-water (l kg ⁻¹)	X		K _{oc}
Partition coefficient solid-water in soil (l kg ⁻¹)		X	K _{psoil}
Soil-water partition coefficient (m ³ m ⁻³)		X	K _{soil-water}
Pseudo first-order rate constant for volatilisation from soil (d)		X	k _{volat}
Pseudo first-order rate constant for leaching from soil (d)		X	k _{leach}
Half-life for biodegradation in soil (d)	X		DT50
Pseudo first-order rate constant for biodegradation in soil (d)		X	K _{bio_{soil}}
First-order rate constant for removal from top soil (d)		X	k
Bulk density of soil (kg m ⁻³)		X	RHO _{soil}
Annual average total deposition flux (mg m ⁻² d ⁻¹)	X		DEP _{total_{ann}}
Aerial deposition flux per soil volume (mg kg ⁻¹ d ⁻¹)		X	D _{air}
Concentration due to 10 years of continuous deposition (mg kg ⁻¹)		X	C _{dep_{soil 10} (0)}
Effluent discharge rate from STP (l d ⁻¹)		X	ELLUENT _{stp}
Rate of sewage sludge production (kg d ⁻¹)		X	SLUDGERATE
Fraction of emission to sludge by STP (-)	X		F _{stp_{sludge}}
Concentration in dry sewage sludge (mg kg ⁻¹)		X	C _{sludge}
Concentration after the first year of sludge application (mg kg ⁻¹)		X	C _{sludge_{soil 1} (0)}
Fraction accumulation in one year (-)		X	F _{acc}
Initial concentration after 10 years of application mg kg ⁻¹		X	C _{sludge_{soil10} (0)}
Sum of both concentration due to deposition and sludge after 10 years (mg kg ⁻¹)		X	C _{soil 10 (0)}
Initial concentration in steady-state situation (mg kg ⁻¹)		X	C _{soil ∞ (0)}
Fraction of steady-state in soil (-)		X	F _{st - st}
Average concentration in soil over T days (mg kg ⁻¹)		X	C _{local_{soil}}
Predicted environmental concentration in soil (mg kg ⁻¹)		X	PEC _{local_{soil}}
Predicted environmental concentration in soil porewater (mg kg ⁻¹)		X	PEC _{local_{soil, porew}}

A1.2.1 Derivation of removal rate constants

$K_{air-water}$ = Air-water partition coefficient (-)

$$K_{air-water} = \frac{HENRY}{R \times TEMP} \quad (9)$$

HENRY = Henry's Law constant (Pa m⁻³ mol⁻¹) – input data for each substance

R = gas constant (Pa m⁻³ mol⁻¹ k⁻¹) – 8.314

TEM = Temperature at air-water interphase (K) – 285

K_{psoil} = Partition coefficient solid-water in soil (l kg⁻¹)

$$K_{psoil} = FOC_{soil} \times KOC \quad (10)$$

FOC_{soil} = Weight fraction of organic carbon in soil solids (K_{g_{oc}} kg_{solids}) – 0.02

KOC = partition coefficient organic carbon-water (l kg⁻¹) – Input data

$K_{soil-water}$ = Soil-water partition coefficient ($m^3 m^{-3}$):

$$K_{soil-water} = Fair_{soil} \times K_{air-water} + Fwater_{soil} + Fsolid_{soil} \times \frac{Kp_{soil}}{1000} \times RHO_{solid} \quad (11)$$

$Fair_{soil}$ = Fraction air in compartment soil ($m^3 m^{-3}$) – 0.2

$Fwater_{soil}$ = Fraction water in compartment soil ($m^3 m^{-3}$) – 0.2

$Fsolid_{soil}$ = Fraction solids in compartment soil ($m^3 m^{-3}$) – 0.6

RHO_{solid} = density of the solid phase ($kg m^{-3}$) – 2500

K_{volat} = pseudo first-order rate constant for volatilisation from soil (d^{-1}):

$$\frac{1}{k_{volatilisation}} = \left(\frac{1}{kasl_{air} \times K_{air-water}} + \frac{1}{kasl_{soilair} \times K_{air-water} \times kasl_{soilwater}} \right) \times K_{soil-water} \times DEPTH_{soil} \quad (12)$$

$Kasl_{air}$ = partial mass transfer coefficient at air-side of the air-soil interphase
($mg d^{-1}$) – 120

$Kasl_{soilair}$ = partial mass transfer coefficient at soil air-side of the air-soil interphase
($mg d^{-1}$) – 0.48

$Kasl_{soilwater}$ = partial mass transfer coefficient at soilwater -side of the air-soil
interphase ($mg d^{-1}$) – 4.8×10^{-5}

$DEPTH_{soil}$ = mixing depth in soil (m)

Terrestrial ecosystems: 0.2 m

Crops for human consumption: 0.2 m

Grass for cattle: 0.1 m

K_{leach} = pseudo first-order rate constant for leaching from soil (d^{-1}):

$$K_{leach} = \frac{Finf_{soil} \times RAINrate}{K_{soil-water} \times DEPTH_{soil}} \quad (13)$$

$Finf_{soil}$ = fraction of rainwater that infiltrates into soil (-) – 0.25

$RAINrate$ = Rate of wet precipitation (700 mm/year) ($m d^{-1}$) – 1.92×10^{-3}

$k_{bio_{soil}}$ = pseudo first-order rate constant for biodegradation in soil (d^{-1})

See table below for determination of $DT50_{bio_{soil}}$ (half-life for biodegradation in bulk soil (d):

Kp_{soil}	Ready biodegradable	Ready biodegradable Failing 10-days window	Inherent biodegradable
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≤ 100	30	90	300
100 – 1,000	300	900	3,000
>1,000 –10,000	3,000	9,000	30,000
etc.	etc.	etc.	etc.

$$k_{bio_{soil}} = \frac{\ln 2}{DT50_{soil}} \quad (14)$$

k = first-order rate constant for removal from top soil (d^{-1}):

$$k = k_{volat} + k_{leach} + k_{bio_{soil}} \quad (15)$$

A1.2.2 Derivation of the initial concentration after 10 years of sludge application

As a worst case scenario for exposure it is assumed that sludge application takes place over a period of 10 years.

RHO_{soil} = bulk density of soil ($kg\ m^{-3}$):

$$RHO_{soil} = F_{solid_{soil}} \times RHO_{solid} + F_{water_{soil}} \times RHO_{water} + F_{air_{soil}} \times RHO_{air} \quad (16)$$

$F_{solid_{soil}}$ = Fraction of solid phase in soil ($m^3\ m^{-3}$): 0.6

RHO_{solid} = density of solids ($kg\ m^{-3}$): 2500

$F_{water_{soil}}$ = Volume fraction water in soil ($m^3\ m^{-3}$): 0.2

RHO_{water} = Density of water phase ($kg\ m^{-3}$): 1000

$F_{air_{soil}}$ = Volume fraction air in soil ($m^3\ m^{-3}$): 0.2

RHO_{air} = Density of air ($kg\ m^{-3}$): 1.3

D_{air} = aerial deposition flux per kg of soil ($mg\ kg^{-1}\ d^{-1}$):

$$D_{air} = \frac{DEPTH_{total_{ann}}}{DEPTH_{soil} \times RHO_{soil}} \quad (17)$$

$DEPTH_{total_{ann}}$ = annual average total deposition flux ($mg\ m^{-2}\ d^{-1}$): Eq 8

$DEPTH_{soil}$ = mixing depth of soil (m): see eq. 11

$Cdep_{soil\ 10}(0)$ = Concentration due to 10 years of continuous deposition ($mg\ kg^{-1}$):

$$Cdep_{soil\ 10}(0) = \frac{D_{air}}{k} - \frac{D_{air}}{k} \times e^{-365 \times 10 \times k} \quad (18)$$

k = first-order rate constant for removal from top soil: See eq. 15

Sludge application is not a continuous process. The concentration and remaining fractions must therefore be calculated yearly during the 10-year period.

$EFFLUENT_{stp}$ = Effluent discharge rate from STP ($l\ d^{-1}$):

$$\text{EFFLUENT}_{\text{stp}} = \text{CAPACITY}_{\text{stp}} \times \text{WASTEWinhab} \quad (19)$$

$$\text{CAPACITY}_{\text{stp}} (\text{eq}) = 10,000$$

$$\text{WASTEWinhab} (\text{l d}^{-1} \text{eq}^{-1}) = 200$$

SLUDGERATE = Rate of sewage sludge production (kg d^{-1}):

$$\text{SLUDGERATE} = \frac{2}{3} \times \text{SUSPCONC}_{\text{inf}} \times \text{EFFLUENT}_{\text{stp}} + \text{SURPLUSsludge} \times \text{CAPACITY}_{\text{stp}} \quad (20)$$

$$\text{SUSPCONC}_{\text{inf}} = \text{Concentration of suspended matter in STP influent (mg m}^{-3}\text{): } 0.45$$

$$\text{SURPLUSsludge} = \text{Surplus sludge per inhabitant equivalent (kg d}^{-1} \text{eq}^{-1}\text{): } 0.011$$

$$\text{CAPACITY}_{\text{stp}} = \text{Capacity of the STP (eq): } 10000$$

C_{sludge} = Concentration in dry sewage sludge (mg kg^{-1}):

$$C_{\text{sludge}} = \frac{F_{\text{stp sludge}} \times E_{\text{local water}} \times 10^6}{\text{SLUDGERATE}} \quad (21)$$

$F_{\text{stp sludge}}$ = Fraction of emission directed to sludge by STP (-): Input data

$E_{\text{local water}}$ = Local emission rate to water during episode (kg d^{-1}): See eq 1 for water compartment

$C_{\text{sludge soil 1}}(0)$ = Concentration just after the first year of sludge application (mg kg^{-1}):

$$C_{\text{sludge soil 1}}(0) = \frac{C_{\text{sludge}} \times \text{APPL}_{\text{sludge}}}{\text{DEPTH}_{\text{soil}} \times \text{RHO}_{\text{soil}}} \quad (22)$$

$\text{APPL}_{\text{sludge}}$ = Dry sludge application rate ($\text{kg m}^{-2} \text{yr}^{-1}$):

$$\text{PEC}_{\text{local soil}}: 0.5$$

$$\text{PEC}_{\text{local agr. soil}}: 0.5$$

$$\text{PEC}_{\text{local grassland}}: 0.1$$

$\text{DEPTH}_{\text{soil}}$ = mixing depth of soil (m): See eq. 11

RHO_{soil} = Bulk density of soil (kg m^{-3}): See eq. 16

F_{acc} = Fraction accumulation in one year (-):

$$F_{\text{acc}} = e^{-365 \times k} \quad (23)$$

k = first-order rate constant for removal from top soil (d^{-1}): see eq. 15

At the end of each year a fraction F_{acc} of the initial concentration remains in the top soil layer. The initial concentration after 10 years of application is given by:

$$C_{\text{sludge soil 10}}(0) = C_{\text{sludge soil 1}}(0) \times [1 + \sum_{n=1}^9 F_{\text{acc}}^n] \quad (24)$$

The sum of both the concentration due to deposition and sludge is the initial concentration in year 10:

$$C_{\text{soil 10}}(0) = C_{\text{dep soil 10}}(0) + C_{\text{sludge soil 10}}(0) \quad (25)$$

$C_{\text{dep soil 10}}(0)$ = Concentration due to 10 years of continuous deposition (mg kg^{-1}):

see eq. 18.

A1.2.3. Indicating persistency in soil

$C_{soil \infty} (0)$ = Initial concentration in steady-state situation ($mg\ kg^{-1}$):

$$C_{soil \infty} (0) = \frac{D_{air}}{k} + C_{sludge_{soil\ 1}} (0) \times \frac{1}{1-F_{acc}} \quad (26)$$

k = first-order rate constant for removal from top soil (d^{-1}): see eq. 15

D_{air} = areal deposition flux per kg of soil ($mg\ kg^{-1}\ d^{-1}$): see eq. 17

$C_{sludge_{soil\ 1}} (0)$ = Concentration just after the first year of sludge application ($mg\ kg^{-1}$) See eq. 23

F_{acc} = Fraction accumulation in one year (-): See eq. 23.

$F_{st - st}$ = Fraction of steady-state in soil achieved (-):

$$F_{st - st} = \frac{C_{soil\ 10}(0)}{C_{soil \infty} (0)} \quad (27)$$

$C_{local\ soil}$ = Average concentration in soil over T days

$$C_{local\ soil} = \frac{D_{air}}{k} + \frac{1}{kT} [C_{soil} (0) - \frac{D_{air}}{k}] \times [1 - e^{-kT}] \quad (28)$$

D_{air} = areal deposition flux per kg of soil ($mg\ kg^{-1}\ d^{-1}$): see eq. 17

k = first-order rate constant for removal from top soil (d^{-1}): see eq. 15

T = Averaging time (d):

PEC $_{local\ soil}$: 30

PEC $_{local\ agr.\ soil}$: 180

PEC $_{local\ grassland}$: 180

$C_{soil} (0)$ = Initial concentration after sludge application ($mg\ kg^{-1}$): See eq. 25

A1.2.4 PEC calculations for soil and porewater

PEC $_{local\ soil}$ = Predicted environmental concentration in soil ($mg\ kg^{-1}$):

$$PEC_{local\ soil} = C_{local\ soil} + PEC_{regional\ natural\ soil} \quad (29)$$

PEC $_{regional\ natural\ soil}$ ($mg\ kg^{-1}$): Regional concentration in natural soil

PEC $_{local\ soil, porewater}$ = Predicted environmental concentration in porewater ($mg\ l^{-1}$):

$$PEC_{local\ soil, porewater} = \frac{PEC_{local\ soil} \times RHO_{soil}}{K_{soil-water} \times 1000} \quad (30)$$

$K_{soil-water}$ = Soil-water partition coefficient ($m^3\ m^{-3}$): see eq. 11

RHO_{soil} = bulk density of soil ($kg\ m^{-3}$): See eq. 16.

A1.2.5 PEC calculations for groundwater compartment

PEC_{local,grw} = predicted environmental concentration in groundwater (mg l⁻¹):

$$\text{PEC}_{\text{local,grw}} = \text{PEC}_{\text{local,agr soil porew}} \quad (31)$$

PEC_{local,agr soil porew} = predicted environmental concentration in porewater (mg l⁻¹):

see eq. 30

A1.3 Aquatic compartment

Table A1.3: Elements, input data and calculated output to PEC_{local} for the aquatic compartment.

Elements	Input data	Output calculations	Term
Concentration in untreated wastewater (mg l ⁻¹)		X	C _{local,inf}
Fraction of emission to water from STP (-)	X		F _{stp,water}
Concentration in the STP effluent (mg l ⁻¹)		X	C _{local,eff}
Partition coefficient organic carbon-water (l kg ⁻¹)	X		K _{oc}
Solid-water partition coefficient of suspended matter (l kg ⁻¹)		X	K _{p,susp}
Local concentration in surface water during emission episode (mg l ⁻¹)		X	C _{local,water}
Days of emission (d yr ⁻¹)	X		T _{emission}
Annual average concentration in surface water (mg l ⁻¹)		X	C _{local,water,ann}
Predicted environmental concentration during episode (mg l ⁻¹)		X	PEC _{local,water}
Annual average predicted environmental concentration (mg l ⁻¹)		X	PEC _{local,water,ann}
Regional concentration in water (mg m ⁻³)	X		PEC _{regional,water}

C_{local,inf} = Concentration in untreated wastewater mg l⁻¹)

$$\text{C}_{\text{local,inf}} = \frac{\text{E}_{\text{local,water}} \times 10^6}{\text{Effluent}_{\text{stp}}} \quad (32)$$

E_{local,water} = Local emission rate to wastewater during episode (kg d⁻¹): See eq 1 for the aquatic compartments

Effluent_{stp} = Effluent discharge rate at STP (l d⁻¹): see eq. 19

C_{local,eff} = Concentration of substance in the STP effluent (mg l⁻¹):

$$\text{C}_{\text{local,eff}} = \text{C}_{\text{local,inf}} \times \text{F}_{\text{stp,water}} \quad (33)$$

F_{stp,water} = Fraction of emission directed to water by STP (-): Input data

K_{p,susp} = solids-water partition coefficient of suspended matter (l kg⁻¹):

$$\text{K}_{\text{p,susp}} = \text{F}_{\text{oc,susp}} \times \text{K}_{\text{oc}} \quad (34)$$

K_{oc} = partition coefficient organic carbon-water (l kg⁻¹): Input data for each substance

FoC_{susp} = weight fraction of organic carbon in compartment water (kg kg⁻¹): 0.1

Clocal_{water} = local concentration in surface water during emission episode (mg l⁻¹):

$$C_{local,water} = \frac{C_{local,eff}}{(1 + K_{p,susp} \times SUSP_{water} \times 10^6) \times DILUTION} \quad (35)$$

SUSP_{water} = Concentration of suspended matter in the river (mg l⁻¹): 15

DILUTION = Dilution factor (-): 10

Alternatively DILUTION can be determined based on relevant data:

$$DILUTION = \frac{EFFLUENT_{stp} + FLOW}{EFFLUENT_{stp}} \quad (36)$$

FLOW = Flow rate of river (l d⁻¹): Input from data set

Clocal_{water,ann} = Annual average concentration in surface water (mg l⁻¹):

$$C_{local,water,ann} = C_{local,water} \times \frac{T_{emission}}{365} \quad (37)$$

T_{emission} = Number of days per year the emission takes place (d): Input data

PEClocal_{water} = Predicted environmental concentration during episode (mg l⁻¹):

$$PEC_{local,water} = C_{local,water} + PEC_{regional,water} \quad (38)$$

PEClocal_{water,ann} = Annual average predicted environmental concentration (mg l⁻¹):

$$PEC_{local,water,ann} = C_{local,water,ann} + PEC_{regional,water} \quad (39)$$

PEC_{regional,water} = Regional concentration in surface water (mg l⁻¹): Input data

A1.4 Sediment compartment

Table A1.4: Elements, input data and calculated output to PEC_{local} for the sediment compartment.

Elements	Input data	Output calculations	Term
Partition coefficient organic carbon-water (l kg ⁻¹)	X		K _{oc}
Solid-water partition coefficient of suspended matter (l kg ⁻¹)		X	K _{p_{susp}}
Suspended matter-water partition coefficient (m ³ m ⁻³)		X	K _{susp-water}
Concentration in surface water during episode	X		PEC _{local_{water}}
Bulk density of suspended matter (kg m ⁻³)		X	RHO _{susp}
Predicted environmental concentration in sediment (mg kg ⁻¹)		X	PEC _{local_{sed}}

In this section the local concentration in sediment during episode is derived. PEC_{local} for sediment can be compared to PNEC for sediment-dwelling organisms.

K_{p_{susp}} = Solid-water partition coefficient of suspended matter (l kg⁻¹):

$$K_{p_{susp}} = F_{OC_{susp}} \times K_{oc} \quad (40)$$

K_{oc} = partition coefficient organic carbon-water (l kg⁻¹): Input data

F_{OC_{susp}} = Weight fraction of organic carbon in sediment solids (kg kg⁻¹): 0.05

K_{susp-water} = Suspended matter-water partition coefficient (m³ m⁻³):

$$K_{susp-water} = K_{air-water} + F_{water_{sed}} + F_{solids_{sed}} \times \frac{K_{p_{susp}}}{1000} \times RHO_{solids} \quad (41)$$

F_{water_{sed}} = fraction water in sediment compartment (m³ m⁻³): 0.8

F_{solids_{sed}} = fraction solids in sediment compartment (m³ m⁻³): 0.2

RHO_{solids} = Density of the solid phase (kg m⁻³): 2,500

K_{air-water} = Air-water partition coefficient (-). See eq. 9

RHO_{susp} = Bulk density of suspended matter (kg m⁻³):

$$RHO_{susp} = F_{solid_{susp}} \times RHO_{solid} + F_{water_{susp}} \times RHO_{water} \quad (42)$$

F_{solid_{susp}} = Volume fraction solids in suspended matter (m³ m⁻³): 0.1

RHO_{solid} = density of the solid phase (kg m⁻³): 2,500

F_{water_{susp}} = Volume fraction water in suspended matter (m³ m⁻³): 0.9

RHO_{water} = density of the water phase (kg m⁻³): 1,000

PEC_{local_{sed}} = Predicted environmental concentration in sediment (mg kg⁻¹):

$$PEC_{local_{sed}} = \frac{K_{susp-water}}{RHO_{susp}} \times PEC_{local_{water}} \times 1,000 \quad (43)$$

PEC_{local_{water}} = Predicted environmental concentration during episode (mg l⁻¹):

See eq. 38

Substance	Abbr.	CAS no.	Persistence (abiotic)		Biodegradation			Bioaccumulation		Toxicity				
			Hydrolysis	Photodegradation	Primary	Ultimate	Ready biodegradable	Octanol-water	Bioconcentration	Algae	Daphnids	Fish	PNEC	PNEC
				Half life (days)										
2-ethanolamine	MEA	141-43-5	No data	0,3 days	3,9221 (days)	3,2486 (weeks)	Yes	-1,61	0,8953	411	217	2271	217	0,217
3-aminopropanol	AP	156-87-6	No data	0,3 days	3,9121 (days)	3,2176 (weeks)	Yes	-1,12	0,8968	227	134	1621	134	0,134
4-amino-1-butanol	AB	13325-10-5	No data	No data	No data	No data	No data	No data	No data	No data	No data	No data	No data	No data
1-amino-2-propanol	MIPA	78-96-6	No data	0,3 days	3,9121 (days)	3,2176 (weeks)	Yes	-1,19	0,8989	256	149	1812	149	0,149
Diglycolamine	DGA	929-06-6	No data	0,2 days	3,8590 (days)	3,1426 (weeks)	Yes	-1,89	0,8934	1105	548	7224	548	0,548
2-methylaminoethanol	MMEA	109-83-1	No data	0,1 days	3,9121 (days)	3,2176 (weeks)	Yes	-1,15	0,9007	237	139	1684	139	0,139
2-ethylaminoethanol	EAE	110-73-6	No data	0,1 days	3,8919 (days)	3,1866 (weeks)	Yes	-0,66	0,9087	126	83	951	83	0,083
Diethanolamine	DEA	111-42-2	No data	0,1 days	3,9981 (days)	3,3112 (days-weeks)	Yes	-1,71	0,8944	834	430	5560	430	0,43
Diisopropanolamine	DIPA	110-97-4	No data	0,1 days	3,9578 (days)	3,2492 (weeks)	Yes	-0,88	0,9003	272	170	1991	170	0,17
N-(2-hydroxyethyl)ethylenediamine	AEEA	111-41-1	No data	0,09 days	3,9135 (days)	3,1779 (weeks)	Yes	-2,13	0,8934	1617	759	10282	759	0,759
N,N'-bis(2-hydroxyethyl)ethylenediamine	BHE	4439-20-7	No data	0,06 days	3,9794 (days)	3,2405 (weeks)	Yes	-2,23	0,8933	2714	1244	17057	1244	1,244
N,N-Dimethylethanolamine	DMMEA	108-01-0	No data	0,1 days	3,5606 (days-weeks)	2,9074 (weeks)	Yes	-0,94	0,8953	199	123	1452	123	0,123
N-methyldiethanolamine	MDEA	105-59-9	No data	0,1 days	3,6467 (days-weeks)	3,0010 (weeks)	Yes	-1,5	0,8936	676	363	4579	363	0,363
Diethylaminoethanol	DEEA	100-37-8	No data	0,1 days	3,5201 (days-weeks)	3,8454 (weeks)	Yes	-0,05	0,9225	53	41	432	41	0,041
Triethanolamine	TEA	102-71-6	No data	0,1 days	3,7328 (days-weeks)	3,0946 (weeks)	Yes	-1	0,8941	4092	1771	25006	1771	1,771
Dimethylpropanolamine	DMPA	3179-63-3	No data	0,1 days	3,5403 (days-weeks)	2,8764 (weeks)	Yes	-0,44	0,9005	104	72	799	72	0,072
2-Amino-2-methylpropanol	AMP	124-68-5	No data	0,4 days	3,7384 (days-weeks)	2,9745 (weeks)	Yes	-0,74	0,9046	145	94	1083	94	0,094
2-Amino-2-methyl-1,3-propanediol	AMPD	115-69-5	No data	0,4 days	3,8448 (days)	3,0991 (weeks)	Yes	-1,1	0,896	305	182	2184	182	0,182
2-Amino-2-ethyl-1,3-propanediol	AEPD	115-70-8	No data	0,3 days	3,8246 (days)	3,0681 (weeks)	Yes	-0,6	0,9044	156	104	1177	104	0,104
N-tertbutylethanolamine	TBEA	4620-70-6	No data	0,1 days	3,6979 (days-weeks)	2,9125 (weeks)	Yes	0,41	1,123	40	32	332	32	0,032
Ethylenediamine	EDA	107-15-3	No data	0,2 days	3,8476 (days)	3,1152 (weeks)	Yes	-2,04	0,8936	409	215	2752	215	0,215
1,3-Propanediamine	PDA	109-76-2	No data	0,2 days	3,8274 (days)	3,0842 (weeks)	Yes	-1,43	0,8957	227	134	1615	134	0,134
Neopentanediamine	DMPDA	7328-91-8	No data	0,2 days	3,6334 (days-weeks)	2,8191 (weeks)	Yes	-0,26	0,9438	76	55	596	55	0,055
1-Amino-1-methylaminopropane	MAPA	6291-84-5	No data	0,1 days	3,8071 (days)	3,0532 (weeks)	Yes	-0,66	0,9129	126	83	949	83	0,083
Diethylenetriamine	DETA	111-40-0	No data	0,07 days	3,8237 (days)	3,0445 (weeks)	Yes	-2,13	0,8936	1618	758	10281	758	0,758
3-(2-Aminoethyl)aminopropylamine	PETA	13531-52-7	No data	0,07 days	3,8085 (days)	3,0135 (weeks)	Yes	-1,64	0,895	827	434	5556	434	0,434
N-(3-aminopropyl)1,4-butanediamine	Spermid	124-20-9	No data	0,07 days	3,768 (days)	2,9515 (weeks)	Yes	-0,66	0,9137	207	136	1558	136	0,136
N,N'-bis(3-Aminopropyl)-1,4-butanediamine	Spermin	71-44-3	No data	0,05 days	3,7289 (days-weeks)	2,8498 (weeks)	Yes	-0,68	0,9139	300	196	2447	196	0,196
1-Amino-1-cyclohexylaminopropane	ACHP	3312-60-5	No data	0,08 days	3,7088 (days-weeks)	2,9027 (weeks)	Yes	1,61	5,062	6	6	54	6	0,006
Dimethylaminopropylamine	DMAPA	109-55-7	No data	0,1 days	3,4556 (days-weeks)	2,7430 (weeks-months)	No	-0,45	0,9087	104	72	799	72	0,072
Tetra-N-methyl-propanedioldiamine	TMDPA	110-95-2	No data	0,07 days	3,0838 (weeks)	2,4018 (weeks-months)	No	0,23	0,9253	44	35	366	35	0,035
N-[3-(Dimethylamino)propyl]-N,N-dimethyl-1,3-propanediamine	TMBPA	6711-48-4	No data	0,04 days	3,0447 (weeks)	2,3000 (weeks-months)	No	0,2	0,9423	66	53	545	53	0,053
Piperazine	PZ	110-85-0	No data	0,06 days	3,8100 (days)	3,0557 (weeks)	Yes	-1,5	0,8957	194	58	1141	58	0,058
1-(2-Hydroxyethyl)piperazine	EtOH-PZ	103-76-4	No data	0,06 days	3,5446 (days-weeks)	2,8411 (weeks)	Yes	-1,56	0,8935	807	431	5470	431	0,431
1-(2-Aminoethyl) piperazine	AE-PZ	140-31-8	No data	0,05 days	3,4599 (days-weeks)	2,7077 (weeks-months)	No	-1,57	0,5	809	431	5480	431	0,431
Morpholine	Morph	110-91-8	No data	0,08 days	3,7556 (days)	3,0224 (weeks)	Yes	-0,86	0,9032	106	71	804	71	0,071
Piperidine	Piper	110-89-4	No data	0,1 days	3,7682 (days)	3,0354 (weeks)	Yes	0,84	1,56	6	6	56	6	0,006
2-piperidineethanol	2-Piper-ETOH	1484-84-0	No data	0,1 days	3,8341 (days)	3,0981 (weeks)	Yes	0,63	0,5	23	20	197	20	0,02
1-(2-Hydroxyethyl)piperidine	EtOH-Piper	3040-44-6	No data	0,1 days	3,5028 (days-weeks)	2,8188 (weeks)	Yes	0,96	1,207	32	27	269	27	0,027
Pyrrolidine	Pyrrol	123-75-1	No data	0,1 days	3,7884 (days)	3,0664 (weeks)	Yes	0,46	1,16	11	10	98	10	0,01
Alanine	Ala	56-41-7	No data	0,3 days	4,1480 (days)	3,3913 (days-weeks)	Yes	-2,96	0,893	56411	21693	325000	21693	21,693
Sarcosine	Sarc	107-97-1	No data	0,2 days	4,1480 (days)	3,3913 (days-weeks)	Yes	-2,78	0,8931	No data	No data	No data	No data	No data
Glycine	Glyc	56-40-6	No data	0,4 days	4,1683 (days)	3,4223 (days-weeks)	Yes	-3,21	0,893	93478	32749	515000	32749	32,749
Dimethylamine	DMA	124-40-3	No data	0,2 days	3,8260 (days)	3,1240 (weeks)	Yes	-0,38	0,9306	29	21	232	21	0,021
Triethylamine	TEA	121-44-8	No data	0,1 days	3,4137 (days-weeks)	2,7207 (weeks-months)	No	1,45	2,689	4	5	41	4	0,004
Tetrahydrothiophenedioxide	Sulfolane	126-33-0	No data	0,8 days	3,6744 (days-weeks)	2,9336 (weeks)	Yes	-0,77	0,9011	1473	4644	10054	1473	1,473

Median
Highest toxicity
Lowest toxicity

PNEC
Median
Lowest
Highest

134
4
32749

0,134
0,004
32,749

Substance	Abbr.	CAS no.	Persistence (abiotic)		Biodegradation			Bioaccumulation		Toxicity				
			Hydrolysis	Photodegradation Half life (days)	Primary Estimated time factor	Ultimate Estimated time factor	Ready biodegradable Yes/No	Octanol-water logPow	Bioconcentration BCF	Algae (EC50 (mg/L))	Daphnids EC50(mg/L)	Fish LC50(mg/L)	PNEC µg/L	PNEC (mg/L)
Acetic acid		64-19-7	No data	17,2	4,1467 (days)	3,4311 (days-weeks)	Yes	-0,17	0,7494	4403	12270	25786	4403	4,403
Oxalic acid		144-62-7	No data	10,3	4,4890 (hours-days)	3,7294 (days-weeks)	Yes	-1,74	0,894	4403	12270	25786	4403	4,40
Bicine		150-25-4	No data	0,1	3,9688 (days)	3,2683 (days-weeks)	Yes	-3,27	0,893	164000	58956	913000	58956	58,96
1-hydroxythane-1,1-phosphonic acid	HEPD	2809-21-4	No data	8,8	3,3970 (days-weeks)	2,5318 (weeks-months)	No	-0,01	0,9172	No data*	No data*	No data*	No data	No data
N-(2-hydroxyethyl)glycine	HeGly	5835-28-9	No data	No data	No data	No data	No data	No data	No data	No data	No data	No data	No data	No data
Ammonia		7664-41-7	No data	Not relevant	Not relevant	Not relevant	Not relevant	Not relevant	Not relevant	100	263	545	100	0,1
Formaldehyde		50-00-0	No data	1,3	4,0011 (days)	3,1551 (weeks)	Yes	0,35	1,056	48	46	13	13	0,013
Acetaldehyde		75-07-0	No data	0,6	3,9808 (days)	3,1241 (weeks)	Yes	-0,34	0,9265	152	163	34	34	0,034
Ethylene glycol		107-21-1	No data	1,3	4,0171 (days)	3,3819 (days-weeks)	Yes	-1,36	0,894	3536	16104	38110	3536	3,536
Acetone		67-64-1	No data	52,4	3,7417 (days-weeks)	3,0483 (weeks)	Yes	-0,24	0,929	4852	2241	711	711	0,711
Acetonitrile		75-05-8	No data	414	3,7233 (days-weeks)	3,0261 (weeks)	Yes	-0,34	0,9244	436	1327	2850	436	0,436
Methylamine		74-89-5	No data	0,5	3,8462 (days)	3,1550 (weeks)	Yes	-0,57	0,9144	43	28	323	28	0,028
Dimethylamine		124-40-3	No data	0,2	3,8260 (days)	3,1240 (weeks)	Yes	-0,38	0,9306	29	21	232	21	0,021
Ethylamine		75-04-7	No data	0,4	3,8260 (days)	3,1240 (weeks)	Yes	-0,13	0,9559	28	21	223	21	0,021
Diethylamine		109-89-7	No data	0,1	3,7855 (days)	3,0620 (weeks)	Yes	0,58	1,262	10	9	85	9	0,009
Ethyl-methylamine		624-78-2	No data	0,1	3,8057 (days)	3,0930 (weeks)	Yes	0,15	1,026	17	14	145	14	0,014
Propylamine		107-10-8	No data	0,3	3,8057 (days)	3,0930 (weeks)	Yes	0,48	1,167	17	14	139	14	0,014
2-methyl-2-(methylamino)propane-1-ol		27646-80-6	No data	No data	No data	No data	No data	No data	No data	No data	No data	No data	No data	No data
Nitromethane		75-52-5	No data	1,3	3,7597 (days)	3,0643 (weeks)	Yes	-0,35	0,9181	545	1592	3385	545	0,545
Nitroethane		79-24-3	No data	71,8	3,7394 (days-weeks)	3,0333 (weeks)	Yes	0,18	0,9914	306	742	1508	306	0,306
N-(2-hydroxyethyl)-ethylenediamine (HEED)	HEED	111-41-1	No data	0,09	3,9135 (days)	3,1779 (weeks)	Yes	-2,13	0,8934	1617	758	10282	758	0,758
Formamide		75-12-7	No data	5,3	3,9882 (days)	3,0454 (weeks)	Yes	-1,51	0,8936	74	29875	5140	74	0,074
Acetamide		60-35-5	No data	5,4	3,9629 (days)	3,0114 (weeks)	Yes	-1,26	0,8941	51	15220	3220	51	0,051
N-(2-hydroxyethyl)acetamide	HEA	142-26-7	No data	0,7	4,0338 (days)	3,0770 (weeks)	Yes	-1,67	0,8934	185	77427	12972	185	0,185
Hydroxyethylamine acetamide	HEHEAA	44236-39-5	No data	No data	No data	No data	No data	No data	No data	No data	No data	No data	No data	No data
N,N'-bis(2-hydroxyethyl)oxamide	BHEOX	1871-89-2	No data	0,4	4,2333 (hours-days)	3,0214 (weeks)	Yes	-3,06	0,893	No data*	No data*	No data*	No data	No data
N-(2-hydroxyethyl)-formamide (HEF)	HEF	693-06-1	No data	0,5	4,0541 (days)	3,1080 (weeks)	Yes	-2,12	0,8931	303	172000	23462	303	0,303
Piperazine	PZ	110-85-0	No data	0,06 days	3,8100 (days)	3,0557 (weeks)	Yes	-1,5	0,8957	194	58	1141	58	0,058
4-(2-hydroxyethyl)piperazinone	HEPO	23936-04-1	No data	No data	No data	No data	No data	No data	No data	No data	No data	No data	No data	No data
Morpholine	MOR	110-91-8	No data	0,08 days	3,7556 (days)	3,0224 (weeks)	Yes	-0,86	0,9032	106	71	804	71	0,071
4-Acetylmorpholine		1696-20-4	No data	0,2	3,8571 (days)	2,8509 (weeks)	Yes	-0,87	0,8963	74	18051	4366	74	0,074
Imidazol		288-32-4	No data	0,3	3,7495 (days-weeks)	3,0487 (weeks)	Yes	-0,08	0,966	0,28	4,5	44,9	0,28	0,0028
N-(2-hydroxyethyl)imidazole (HEI)	HEI	1615-14-1	No data	0,3	3,8154 (days)	3,1113 (weeks)	Yes	-0,37	0,9268	0,11	11	135	0,11	0,00011
1-(2-hydroxyethyl)-2-imidazolidinone (HEIA)	HEIA	3699-54-5	No data	0,6	3,7894 (days)	3,0715 (weeks)	Yes	-1,5	0,8936	5	34917	28201	5	0,005
Pyrrrole		109-97-7	No data	0,1	3,7509 (days)	3,0509 (weeks)	Yes	0,75	1,456	16	3	15	3	0,003
1,1'-(1,3-phenylene)bis-1H-pyrrrole-2,5-dione		79-24-3	No data	0,2	3,7394 (days-weeks)	3,0333 (weeks)	Yes	0,18	0,9914	306	742	1508	306	0,306
Pyrazine		290-37-9	No data	46,5	3,7322 (days-weeks)	3,0222 (weeks)	Yes	-0,26	0,9444	741	2186	4657	741	0,741
Methylpyrazine		109-08-0	No data	14,5	3,6434 (days-weeks)	2,9163 (weeks)	Yes	0,21	1,041	364	871	1765	364	0,364
Dimethylpyrazine		123-32-0	No data	10,6	3,5547 (days-weeks)	2,8105 (weeks)	Yes	0,63	1,27	175	340	654	175	0,175
Oxazolidone		497-25-6	No data	0,9	3,9157 (days)	2,9600 (weeks)	Yes	-0,16	0,9065	0,4	388	454	0,4	0,0004
4,4-dimethyloxazolidone		51200-87-4	No data	0,1	3,5819 (days-weeks)	2,7793 (weeks)	Yes	-0,08	0,9611	56	42	452	42	0,042
N-nitrosodiethanolamine (NDELA)	NDELA	1116-54-7	No data	0,4	3,9316 (days)	2,8376 (weeks)	Yes	-1,28	0,894	525	300	3679	300	0,3
Nitrosopiperidine (NPIP)	NPIP	100-75-3	No data	No data	No data	No data	No data	No data	No data	No data	No data	No data	No data	No data
Nitrosodiethylamine (NDEA)	NDEA	55-18-5	No data	0,6	3,7189 (days-weeks)	2,5883 (weeks-months)	No	0,48	1,063	29	24	240	24	0,024
Nitrosodimethylamine (NDMA)	NDMA	62-75-9	No data	4,2	3,7593 (days)	2,6503 (weeks-months)	No	-0,57	0,9035	102	66	771	66	0,066
Nitroso-N-methylethylamine (NMEA)	NMEA	10595-95-6	No data	1,1	3,7391 (days-weeks)	2,6193 (weeks-months)	No	0,04	0,9471	55	40	436	40	0,04
Nitrosomorpholine (NMOR)	NMOR	59-89-2	No data	0,1	3,6889 (days-weeks)	2,5488 (weeks-months)	No	-0,44	0,9034	113	79	875	79	0,079
Nitroso-N-propylamine (NDPA)	NDPA	621-64-7	No data	0,5	3,6784 (days-weeks)	2,5263 (weeks-months)	No	1,36	2,42	7	8	69	7	0,007
Nitrosopyrrolidine (NPYR)	NPYR	930-55-2	No data	0,7	3,7218 (days-weeks)	2,5928 (weeks-months)	No	-0,19	0,9162	34	27	279	27	0,027
Nitrosopiperazine (NPZ)	NPZ	5632-47-3	No data	0,1	3,7434 (days-weeks)	2,5840 (weeks-months)	No	0,18	0,9907	51	43	432	43	0,043
Dinitrosopiperazine (DNPZ)	DNPZ	140-79-4	No data	0,3	3,6767 (days-weeks)	2,1104 (months)	No	-0,85	0,8957	231	150	1724	150	0,15
Nitroso(2-hydroxyethyl)glycine	NO-HeGly	80556-89-4	No data	No data	No data	No data	No data	No data	No data	No data	No data	No data	No data	No data
Dimethylnitramine (DMNA)	DMNA	4164-28-7	No data	2,8	3,7178 (days-weeks)	3,0001 (weeks)	No	-0,52	0,9122	No data*	No data*	No data*	No data	No data
Ethanolnitramine (MEA-NO2)	MEA-NO2	74386-82-6	No data	No data	No data	No data	No data	No data	No data	No data	No data	No data	No data	No data
Methylnitramine (MNA)	MNA	598-57-2	No data	82,3	3,7813 (days)	3,0555 (weeks)	Yes	-1,51	0,8944	432	234	2947	234	0,234
N-nitropiperazine (PZ-NO2)	PZ-NO2	42499-41-2	No data	No data	No data	No data	No data	No data	No data	No data	No data	No data	No data	No data
1-methyl-2-(nitramino)-1-propanol (AMP-NO2)	AMP-NO2	1239666-60-4	No data	No data	No data	No data	No data	No data	No data	No data	No data	No data	No data	No data
Diethylnitramine (DENA)	DENA	7119-92-8	No data	0,6	3,6773 (days-weeks)	2,9381 (weeks)	No	0,46	1,12	No data*	No data*	No data*	No data	No data

*Not related to any existing ECOSAR class definition

PNEC	Median	71	0,071
	Lowest	0,11	0,00011
	Highest	58956	58,956

Name and CAS	Method	Environment	Parameter	Result	UNIT	Project	Laboratory
MEA	Microtox	Diluent	EC50	6-39	mg/L	REACT	SINTEF
141-43-5	Pseudokirchneriella subcapitata	Freshwater	EC50	198	mg/L	NIVA	Review
	Chlorococcales (green algae)	Freshwater	EC50	70	mg/L	NIVA	Review
	Chloromonas paramecium (cryptomonad)	Freshwater	EC50	733	mg/L	NIVA	Review
	Entosiphon sulcatum (flagellate)	Freshwater	LC50	300	mg/L	NIVA	Review
	Skeletonema pseudocostatum	Seawater	EC50	198	mg/L	REACT	SINTEF
	Skeletonema pseudocostatum	Seawater	EC50	83	mg/L	NIVA	Review
	Isichrysis galbana (haptocyte)	Seawater	EC50	80-160	mg/L	NIVA	Review
	Daphnia magna	Freshwater	LC50	100	mg/L	REACT	Review
	Daphnia magna	Freshwater	LC50	84-165	mg/L	NIVA	Review
	Crangon crangon (brown shrimp)	Seawater	LC50	100	mg/L	NIVA	Review
	Carassius auratus (Goldfish)	Freshwater	LC50	190	mg/L	REACT	Review
	Danio rerio (zebrafish)	Freshwater	LC50	4340	mg/L	REACT	Review
	Gambusia affinis (western mosquitofish)	Freshwater	LC50	355	mg/L	REACT	Review
	Lepomis macrochirus (bluegill)	Freshwater	LC50	346	mg/L	REACT	Review
	Oncorhynchus mykes (rainbow trout)	Freshwater	LC50	150	mg/L	REACT	Review
	Goldfish (Carassius auratus)	Freshwater	LC50	170	mg/L	NIVA	Review
	Western mosquito fish (Gambusia affinis)	Freshwater	LC50	338	mg/L	NIVA	Review
	Blue gill (Lepomis macrochirus)	Freshwater	LC50	300-329	mg/L	NIVA	Review
	Rainbow trout (Salmo gairdneri)	Freshwater	LC50	167	mg/L	NIVA	Review
	Zebra fish - eggs (Danio rerio)	Freshwater	LC50	60,3	mg/L	NIVA	Review
	Anacystis aeruginosa (blue-green algae)	Freshwater	LOEC (chronic)	1,6-2,1	mg/L	NIVA	Review
	Scenedesmus quadricauda (green algae)	Freshwater	LOEC (chronic)	0,75-0,97	mg/L	NIVA	Review
	Microcystis aeruginosa (blue-green algae)	Freshwater	LOEC (chronic)	1,6-2,1	mg/L	NIVA	Review
AP	Microtox	Diluent	EC50	12	mg/L	REACT	SINTEF
156-87-6	Skeletonema pseudocostatum	Seawater	EC50	21	mg/L	REACT	SINTEF
	Daphnia magna	Freshwater	LC50	500	mg/L	REACH	
	Ptychocheilus oregonensis (northern squashfish)	Freshwater	LC50	10	mg/L	REACT	Review
	Leuciscus idus (fish)	Freshwater	LC50	500	mg/L	REACH	
AB	Microtox	Diluent	EC50	12	mg/L	REACT	SINTEF
13325-10-5	Skeletonema pseudocostatum	Seawater	EC50	30	mg/L	REACT	SINTEF
MIPA	Microtox	Diluent	EC50	17	mg/L	REACT	SINTEF
78-96-6	Skeletonema pseudocostatum	Seawater	EC50	39	mg/L	REACT	SINTEF
	Daphnia magna	Freshwater	LC50	109	mg/L	REACH	
	Carassius auratus (goldfish)	Freshwater	LC50	220	mg/L	REACT	Review
	Pimephales promela (fathead minnows)	Freshwater	LC50	2520	mg/L	REACT	Review
DGA	Microtox	Diluent	EC50	23	mg/L	REACT	SINTEF
929-06-6	Scenedesmus subspicatus	Freshwater	EC50	202	mg/L	REACH	
	Skeletonema pseudocostatum	Seawater	EC50	493	mg/L	REACT	SINTEF
	Daphnia magna	Freshwater	LC50	>500	mg/L	REACH	
	Leuciscus idus (fish)	Freshwater	LC50	>681	mg/L	REACH	
MMEA	Microtox	Diluent	EC50	12	mg/L	REACT	SINTEF
109-83-1	Microtox	Diluent	EC50	12	mg/L	REACT	SINTEF
	Scenedesmus subspicatus	Freshwater	EC50	28	mg/L	REACH	
	Pseudokirchneriella subcapitata	Freshwater	KOEC/NOEC	3	mg/L	SOLVit	SINTEF
	Skeletonema pseudocostatum	Seawater	EC50	70	mg/L	REACT	SINTEF
	Daphnia magna	Freshwater	LC50	33	mg/L	REACH	
	Daphnia magna	Freshwater	LOEC/NOEC	50	mg/L	REACT	Review
	Daphnia magna	Freshwater	LOEC/NOEC	25	mg/L	REACT	Review
	Danio rerio (zebrafish)	Freshwater	LC50	>100	mg/L	REACH	
EAE	Microtox	Diluent	EC50	18	mg/L	REACT	SINTEF
110-73-6	Pseudokirchneriella subcapitata	Freshwater	EC50	37	mg/L	REACH	
	Skeletonema pseudocostatum	Seawater	EC50	27	mg/L	REACT	SINTEF
	Daphnia magna	Freshwater	EC50	35	mg/L	REACH	
	Pimephales promela (fathead minnows)	Freshwater	LC50	1480	mg/L	REACT	Review
	Leuciscus Idus	Freshwater	LC50	147	mg/L	REACH	
DEA	Microtox	Diluent	EC50	22	mg/L	REACT	SINTEF
111-42-2	Skeletonema pseudocostatum	Seawater	EC50	357	mg/L	REACT	SINTEF
	Daphnia magna	Freshwater	EC50	100	mg/L	REACT	Review
	Calanus finmarchicus	Seawater	LC50	380	mg/L	REACT	SINTEF
	Cypridon (Sheephead minnows)	Freshwater	LC50	540	mg/L	REACT	Review
	Pimephales (Fathead minnows)	Freshwater	LC50	1425	mg/L	REACT	Review

DIPA	Microtox	Diluent	EC50	38	mg/L	REACT	SINTEF
110-97-4	Selenastrum capricornutum	Freshwater	EC50	20	mg/L		
	Skeletonema pseudocostatum	Seawater	EC50	240	mg/L	REACT	SINTEF
	Daphnia magna	Freshwater	EC50	187	mg/L		
	Carassius auratus (goldfish)	Freshwater	LC50	3050	mg/L	REACT	Review
	Salmo gairdneri (fish)	Freshwater	LC50	37	mg/L		
AEEA	Microtox	Diluent	EC50	17	mg/L	REACT	SINTEF
111-41-1	Pseudokirchneriella subcapitata	Freshwater	EC50	98	mg/L	REACH	
	Skeletonema pseudocostatum	Seawater	EC50	920	mg/L	REACT	SINTEF
	Daphnia magna	Freshwater	EC50	>100	mg/L	REACH	
BHE	Microtox	Diluent	EC50	52	mg/L	REACT	SINTEF
4439-20-7	Skeletonema pseudocostatum	Seawater	EC50	528	mg/L	REACT	SINTEF

DMMEA	Microtox	Diluent	EC50	19	mg/L	REACT	SINTEF
108-01-0	Skeletonema pseudocostatum	Seawater	EC50	40	mg/L	CESAR	SINTEF
	Daphnia magna	Freshwater	EC50	112	mg/L	CESAR	SINTEF
	Cyprinus carpio (common carp)	Freshwater	LC50	110	mg/L	REACT	Review
	Pimephales promela (fathead minnows)	Freshwater	LC50	1780	mg/L	REACT	Review
MDEA	Microtox	Diluent	EC50	36	mg/L	REACT	SINTEF
105-59-9	Scenedesmus subcapitatus	Freshwater	EC50	20	mg/L	NIVA	Review
	Skeletonema pseudocostatum	Seawater	EC50	141	mg/L	REACT	SINTEF
	Skeletonema pseudocostatum	Seawater	LOEC/NOEC	73	mg/L	NIVA	Review
	Daphnia magna (water flea)	Freshwater	LC50	230	mg/L	NIVA	Review
	Calanus finmarchicus	Seawater	LC50	183	mg/L	REACT	SINTEF
	Pimephales promela (fathead minnows)	Freshwater	LC50	1200	mg/L	NIVA	Review
	Pimephales promela (fathead minnows)	Freshwater	LC50	1000	mg/L	NIVA	Review
	Orfe (Leuciscus Idus)	Freshwater	LC50	100-1200	mg/L	NIVA	Review
DEEA	Microtox	Diluent	EC50	22	mg/L	REACT	SINTEF
100-37-8	Pseudokircheriella subcapitata	Freshwater	EC50	161	mg/L	iCAP	SINTEF
	Skeletonema pseudocostatum	Seawater	EC50	23	mg/L	iCAP	SINTEF
	Skeletonema pseudocostatum	Seawater	EC50	34	mg/L	REACT	SINTEF
	Daphnia magna	Freshwater	EC50	406	mg/L	iCAP	SINTEF
	Acartia tonsa	Seawater	EC50	67	mg/L	iCAP	SINTEF
TEA	Desmodesmus subspicatus (algae)	Freshwater	EC50	216	mg/L	ECHA Dossier	
102-71-6	Ceriodaphnia dubia (invertebrate)	Freshwater	EC50	610	mg/L	ECHA Dossier	
	Pimephales promelas (fish)	Freshwater	LC50	11800	mg/L	ECHA Dossier	
DMPA	Desmodesmus subspicatus	Freshwater	EC50	28	mg/L	ECHA Dossier	
3179-63-3	Skeletonema pseudocostatum	Seawater	EC50	16	mg/L	REACT	SINTEF
	Daphnia magna	Freshwater	EC50	112	mg/L	ECHA Dossier	
	Leuciscus idus (fish)	Freshwater	LC50	147	mg/L	ECHA Dossier	
1DMA2P	Desmodesmus subspicatus	Freshwater	EC50	77	mg/L	ECHA Dossier	
108-16-7	Desmodesmus subspicatus	Freshwater	NOEC	42	mg/L	ECHA Dossier	
	Daphnia magna	Freshwater	EC50	79	mg/L	ECHA Dossier	
	Leuciscus idus (fish)	Freshwater	LC50	148	mg/L	ECHA Dossier	
AMP	Microtox	Diluent	EC50	20	mg/L	REACT	SINTEF
124-68-5	Pseudokircheriella subcapitata	Freshwater	EC50	711	mg/L	CESAR	SINTEF
	Pseudokirchneriella subcapitata	Freshwater	EC50	119	mg/L	NIVA	Review
	Skeletonema pseudocostatum	Seawater	EC50	119	mg/L	CESAR	SINTEF
	Skeletonema pseudocostatum	Seawater	LOEC/NOEC	65	mg/L	NIVA	Review
	Daphnia magna	Freshwater	EC50	325	mg/L	CESAR	SINTEF
	Daphnia sp.	Freshwater	EC50	3332	mg/L	SOLVit	SINTEF
	Daphnia sp.	Freshwater	NOEC	33	mg/L	SOLVit	SINTEF
	Daphnia sp.	Freshwater	NOEC	100	mg/L	NIVA	Review
	Lepomis macrochirus (fish)	Freshwater	LC50	200	mg/L	REACH	
	Pleuronectes platessa (fish)	Seawater	LC50	193	mg/L	REACH	
	Blue gill (Lepomis macrochirus)	Freshwater	NOEC	100	mg/L	REACT	Review
	Lepomis idus	Freshwater	NOEC	320	mg/L	REACT	Review
AMPD	Microtox	Diluent	EC50	30	mg/L	REACT	SINTEF
115-69-5	Pseudokirchneriella subcapitata	Freshwater	EC50	158	mg/L	REACH	
	Skeletonema pseudocostatum	Seawater	EC50	249	mg/L	REACT	SINTEF
	Daphnia magna	Freshwater	EC50	316	mg/L	REACH	
	Danio rerio (zebrafish)	Freshwater	LC50	>10000	mg/L	REACH	
AEPD	Microtox	Diluent	EC50	32	mg/L	REACT	SINTEF
115-70-8	Pseudokirchneriella subcapitata	Freshwater	EC50	158	mg/L	REACH	
	Skeletonema pseudocostatum	Seawater	EC50	78	mg/L	REACT	SINTEF
	Daphnia magna	Freshwater	EC50	668	mg/L	REACH	
	Leuciscus idus melanotus	Freshwater	LC50	460	mg/L	REACH	
TBEA	Skeletonema pseudocostatum	Seawater	EC50	51	mg/L	REACT	SINTEF
4620-70-6							
TBAB	Pseudokirchneriella subcapitata	Freshwater	EC50	35	mg/L	iCAP	SINTEF
1643-19-2	Skeletonema pseudocostatum	Seawater	EC50	570	mg/L	iCAP	SINTEF
	Daphnia magna	Freshwater	EC50	17	mg/L	iCAP	SINTEF
	Acartia tonsa	Seawater	EC50	1048	mg/L	iCAP	SINTEF

EDA	Microtox	Diluent	EC50	13	mg/L	REACT	SINTEF
107-15-3	Skeletonema pseudocostatum	Seawater	EC50	111	mg/L	REACT	SINTEF
	Daphnia magna	Freshwater	EC50	16	mg/L	REACT	Review
	Pimephales promelas (fathead minnows)	Freshwater	LC50	230	mg/L	REACT	Review
	Salmo trutta (brown salmon)	Freshwater	LC50	230	mg/L	REACT	Review
PDA	Desmodesmus subspicatus	Freshwater	EC50	175	mg/L	REACH	
109-76-2	Skeletonema pseudocostatum	Seawater	EC50	299	mg/L	REACT	SINTEF
	Daphnia magna	Freshwater	EC50	27	mg/L	REACH	
	Leuciscus idus (fish)	Freshwater	LC50	>100	mg/L	REACH	

DMPDA 7328-91-8	Skeletonema pseudocostatum	Seawater	EC50	483	mg/L	REACT	SINTEF
	Leuciscus idus (fish)	Freshwater	LC50	147	mg/L	REACH	
MAPA 6291-84-5	Pseudokircheriella subcapitata	Freshwater	EC50	627	mg/L	iCAP	SINTEF
	Skeletonema pseudocostatum	Seawater	EC50	56	mg/L	iCAP	SINTEF
	Skeletonema pseudocostatum	Seawater	EC50	1065	mg/L	CESAR	SINTEF
	Daphnia magna	Freshwater	EC50	116	mg/L	CESAR	SINTEF
	Daphnia magna	Freshwater	EC50	76	mg/L	iCAP	SINTEF
	Acartia tonsa	Seawater	EC50	89	mg/L	iCAP	SINTEF
DETA 111-40-0	Microtox	Diluent	EC50	9	mg/L	REACT	SINTEF
	Skeletonema pseudocostatum	Seawater	EC50	906	mg/L	REACT	SINTEF
	Daphnia magna	Freshwater	EC50	54	mg/L	REACT	Review
	Oryzias latipes (mekada)	Freshwater	LC50	1000	mg/L	REACT	Review
	Poecilia reticulata (guppy)	Freshwater	LC50	1014	mg/L	REACT	Review
PETA 13531-52-7	Desmodesmus subspicatus	Freshwater	EC50	460	mg/L	REACH	
	Skeletonema pseudocostatum	Seawater	EC50	>10000	mg/L	REACT	SINTEF
	Daphnia magna	Freshwater	EC50	26	mg/L	REACH	
	Leuciscus idus (fish)	Freshwater	LC50	>220	mg/L	REACH	
Spermid 124-20-9	Skeletonema pseudocostatum	Seawater	EC50	>10000	mg/L	REACT	SINTEF
Spermin 71-44-3	Skeletonema pseudocostatum	Seawater	EC50	10000	mg/L	REACT	SINTEF
ACHP 3312-60-5	Pseudokirchneriella subcapitata	Freshwater	EC50	9	mg/L	REACH	
	Daphnia magna	Freshwater	EC50	17	mg/L	REACH	
DMAPA 109-55-7	Pseudokirchneriella subcapitata	Freshwater	EC50	34	mg/L	REACH	
	Pseudokirchneriella subcapitata	Freshwater	NOEC	26	mg/L	REACH	
	D. magna	Freshwater	EC50	60	mg/L	REACH	
	Leuciscus idus (fish)	Freshwater	LC50	122	mg/L	REACH	
TMPDA 110-95-2	Pseudokirchneriella subcapitata	Freshwater	EC50	10	mg/L	REACH	
	Pseudokirchneriella subcapitata	Freshwater	NOEC	1	mg/L	REACH	
	D. magna	Freshwater	EC50	53	mg/L	REACH	
	Danio rerio (zebrafish)	Freshwater	LC50	>100	mg/L	REACH	
TMBPA 6711-48-4	Pseudokirchneriella subcapitata	Freshwater	EC50	8	mg/L	REACH	
	Pseudokirchneriella subcapitata	Freshwater	NOEC	1	mg/L	REACH	
	D. magna	Freshwater	EC50	50	mg/L	REACH	
	Danio rerio (zebrafish)	Freshwater	LC50	22	mg/L	REACH	
	Danio rerio (zebrafish)	Freshwater	NOEC	21	mg/L	REACH	
PZ 110-85-0	Microtox	Diluent	EC50	472	mg/L	REACT	SINTEF
	Microtox	Diluent	EC50	13	mg/L	REACT	SINTEF
	Pseudokirchneriella subcapitata	Freshwater	EC50	1271	mg/L	CESAR	SINTEF
	Pseudokirchneriella subcapitata	Freshwater	EC50	472	mg/L	NIVA	Review
	Selenastrum caprocornutum (green algae)	Freshwater	EC50	>1000	mg/L	NIVA	Review
	Skeletonema pseudocostatum	Seawater	EC50	472	mg/L	CESAR	SINTEF
	Skeletonema pseudocostatum	Seawater	EC50	316	mg/L	NIVA	Review
	Daphnia magna	Freshwater	EC50	69	mg/L	CESAR	SINTEF
	Daphnia sp.	Freshwater	EC50	303	mg/L	SOLVit	SINTEF
	Daphnia sp.	Freshwater	NOEC30	30	mg/L	SOLVit	SINTEF
	Daphnia sp.	Freshwater	EC50	10-100	mg/L	NIVA	Review
	Cyprino carpio (carp)	Freshwater	LC50	52-159	mg/L	NIVA	Review
	Poecelia reticulata (guppy)	Freshwater	NOEC	100	mg/L	NIVA	Review
	Kulia sandvicensis (flagtail - bird)	Air	EC50	20	mg/L	NIVA	Review
EtOH-PZ 103-76-4	Microtox	Diluent	EC50	24	mg/L	REACT	SINTEF
	Skeletonema pseudocostatum	Seawater	EC50	329	mg/L	REACT	SINTEF
	Promephales promela (Fathead minnows)	Freshwater	LC50	6410	mg/L	REACT	Review
AE-PZ 140-31-8	Pseudokirchneriella subcapitata	Freshwater	EC50	674	mg/L	SOLVit	SINTEF
	Daphnia sp.	Freshwater	EC50	69	mg/L	SOLVit	SINTEF

MORPH	Microtox	Diluent	EC50	32	mg/L	REACT	SINTEF
110-91-8	Selenastrum tricornutum	Freshwater	EC50	28	mg/L		
	Skeletonema pseudocostatum	Seawater	EC50	9	mg/L	REACT	SINTEF
	Daphnia magna	Freshwater	EC50	101	mg/L	REACT	Review
	Daphnia magna	Freshwater	EC50	119	mg/L	REACT	
	Leuciscus idus (carp)	Freshwater	LC50	263	mg/L	REACT	Review
	Oncorhynchus mykiss (rainbow trout)	Freshwater	LC50	380	mg/L	REACT	Review
	Salmp gaimeri (fish)	Freshwater	LC50	180	mg/L		
PIPER	Microtox	Diluent	EC50	18	mg/L	REACT	SINTEF
110-89-4	Skeletonema pseudocostatum	Seawater	EC50	2	mg/L	REACT	SINTEF
	Artemia saline (brown shrimp)	Seawater	Endpoint (??)10	10	mg/L	REACT	Review
2-PIPER-EtOH	Pseudokirchneriella subcapitata	Freshwater	EC50	44	mg/L	SOLVit	SINTEF
1484-84-0	Daphnia sp.	Freshwater	EC50	202	mg/L	SOLVit	SINTEF
EtOH-PIPER	Pseudokirchneriella subcapitata	Freshwater	EC50	1,6	mg/L	REACH	
3040-44-8	Pseudokirchneriella subcapitata	Freshwater	NOEC	0,3	mg/L	REACH	
	Leuciscus idus	Freshwater	LC50	>100	mg/L	REACH	
PYRROL	Microtox	Diluent	EC50	16	mg/L	REACT	SINTEF
123-75-1	Skeletonema pseudocostatum	Seawater	EC50	3	mg/L	REACT	SINTEF
EtOH-Pyrrol	Pseudokirchneriella subcapitata	Freshwater	EC50	15	mg/L	SOLVit	SINTEF
2955-88-6	Daphnia sp.	Freshwater	EC50	143	mg/L	SOLVit	SINTEF
Ala	Pseudokirchneriella subcapitata	Freshwater	EC50	77	mg/L	iCAP	SINTEF
56-41-7	Skeletonema pseudocostatum	Seawater	EC50	>10000	mg/L	iCAP	SINTEF
	Daphnia magna	Freshwater	EC50	>10000	mg/L	iCAP	SINTEF
	Acartia tonsa	Seawater	EC50	665	mg/L	iCAP	SINTEF
	Danio rerio (zebrafish)	Freshwater	LC50	9	µmol/L		
Sarc	Skeletonema pseudocostatum	Seawater	EC50	>10000	mg/L	CESAR	SINTEF
107-97-1	Daphnia magna	Freshwater	EC50	839	mg/L	CESAR	SINTEF
Glyc	Skeletonema pseudocostatum	Seawater	EC50	3621	mg/L	REACT	SINTEF
56-40-6							
DMA	Selenastrum capricornutum (algae)	Freshwater	EC50	9	mg/L		
124-40-3	Daphnia magna	Freshwater	EC50	48	mg/L		
	Salmo gaimeri (fish)	Freshwater	LC50	17	mg/L		
TeA	Pseudokirchneriella subcapitata	Freshwater	EC50	8	mg/L	REACH	
121-44-8	Pseudokirchneriella subcapitata	Freshwater	NOEC	1	mg/L	REACH	
	Daphnia magna	Freshwater	EC50	34	mg/L	REACH	
	Oncorhynchus mykiss (rainbow trout)	Freshwater	LC50	24	mg/L	REACH	
	Oncorhynchus mykiss (rainbow trout)	Freshwater	NOEC	16	mg/L	REACH	
Sulfolane	Selenastrum capricornutum (algae)	Freshwater	EC50	500	mg/L	REACH	
126-33-0	Daphnia magna	Freshwater	EC50	852	mg/L	REACH	
	Daphnia magna	Freshwater	NOEC	171	mg/L	REACH	
	Oryzias latipes (fish)	Freshwater	LC50	>100	mg/L	REACH	

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Name and CAS	Method	Environment	Conc. (mg/L)	Temp (°C)	ThOD	28 days	Other	Rates coefficients	Half-life (d)	Laboratory
MEA 141-43-5	OECD301D-BOD	Freshwater	2	20		64	ND	0,036488	19,0	SINTEF
	OECD306-BOD	Seawater	2	20		68	ND	0,040694	17,0	SINTEF
	OECD301B-CO2	Activated sludge	19	20		83	ND	0,063284	11,0	REVIEW
	OECD301B-CO2	Activated sludge	20	20		62	ND	0,034557	20,1	Review
	OECD301D-BOD	Freshwater	2	20		78	ND	0,054076	12,8	NTNU
AP 156-87-6	OECD 301C (MITI)-BOD	Mix (sludge, water, etc.)	No information	20		86	ND	0,070218	9,9	REACH
	OECD306-BOD	Seawater	2	20		3	ND	0,001088	637,0	SINTEF
AB 13325-10-5	OECD306-BOD	Seawater	2	20		69	ND	0,041828	16,6	SINTEF
MIPA 78-96-6	OECD301F-manometry	Activated sludge	100	20			d3: 60%	0,305430	2,3	REACH
	OECD306-BOD	Seawater	2	20		58	ND	0,030982	22,4	SINTEF
DGA 929-06-6	OECD301B-DOC	Activated sludge	No information	20		84		0,065449	10,6	REACH
	OECD306-BOD	Seawater	2	20		<1	ND	0,000359	1930,7	SINTEF
MMEA 109-83-1	OECD301A-DOC	Activated sludge	20 mg/L DOC	20			d21: 93%	0,126631	5,5	REACH
	OECD306-BOD	Seawater	2	20		77	ND	0,052488	13,2	SINTEF
EAE 110-73-6	OECD301D-CO2	Activated sludge	10 and 20	20		62		0,034557	20,1	REACH
	OECD306-BOD	Seawater	2	20		70	ND	0,042999	16,1	SINTEF
DEA 111-42-2	OECD301F-manometric	Activated sludge	No data	20		93		0,094974	7,3	REACH
	OECD306-BOD	Seawater	2	20		63	ND	0,035509	19,5	SINTEF
	OECD301D-BOD	Freshwater	2	20		83,2		0,063707	10,9	NTNU
DIPA 110-97-4	OECD301F-manometric	Activated sludge	No data	20		94		0,100479	6,9	REACH
	OECD306-BOD	Seawater	2	20		<1	ND	0,000359	1930,7	SINTEF
AEAA 111-41-1	OECD301F-manometric	Activated sludge	No data	20		45		0,021351	32,5	REACH
	OECD306-BOD	Seawater	2	20		3	ND	0,001088	637,0	SINTEF
BHE 4439-20-7	OECD306-BOD	Seawater	2	20		30	ND	0,012738	54,4	SINTEF
DMMEA 108-01-0	OECD301C-BOD	Mix activ. sludge, water, etc.	100	20			d14: 61%	0,083656	8,3	REACH
	OECD301D-BOD	Freshwater	2	20		86,8		0,072320	9,6	SINTEF
	OECD306-BOD	Seawater	2	20		94		0,100479	6,9	SINTEF
MDEA 105-59-9	OECD301A-DOC	Activated sludge	No data	20			d18: 96%	0,178826	3,9	REACH
	OECD306-BOD	Seawater	2	20		<1	ND	0,000359	1930,7	SINTEF
	OECD301D-BOD	Freshwater	2	20		77,3		0,052957	13,1	NTNU
DEEA 100-37-8	OECD301D-BOD	Activated sludge	No information	20			d10: 82%	0,171480	4,0	REACH
	OECD301D-BOD	Freshwater	2	20		79,2		0,056079	12,4	SINTEF
	OECD306-BOD	Seawater	2	20		2		0,000722	960,5	SINTEF
	OECD306-BOD	Seawater	2	20		<1		0,000359	1930,7	SINTEF
TEA 102-71-6	No information	Activated sludge	168	No information		No information			0,24	REACH
	OECD306-BOD	Seawater	2	20		20	ND	0,007969	87,0	SINTEF
DMPA 3179-63-3	OECD301A-DOC	Activated sludge	No information	20		99		0,164470	4,2	REACH
	OECD306-BOD	Seawater	2	20		16	ND	0,006227	111,3	SINTEF
1DMA2P 108-16-7	OECD301A-DOC	Activated sludge	No information	20		90		0,082235	8,4	REACH
	OECD306-BOD	Seawater	2	20		5	ND	0,001832	378,3	SINTEF
AMP 124-68-5	OECD301F-manometric	Activated sludge	11	20		89		0,078831	8,8	REACH
	OECD301D-BOD	Freshwater	2	20		25,7	ND	0,010609	65,3	SINTEF
	OECD306	Closed bottle (BOD)	2	20		<1	ND	0,000359	1930,7	SINTEF
	Primary deg/LC-MS	Freshwater	0,01	20	Not relevant	97	ND	0,077	9,0	SINTEF
	Primary deg/LC-MS	Freshwater	0,01	10	Not relevant	97	ND	0,077	9,0	SINTEF
	Primary deg/LC-MS	Freshwater	0,01	5	Not relevant	4,3	d56: 97	0,0218	31,8	SINTEF
	OECD301D-BOD	Freshwater	2	20		83,3	ND	0,063920	10,8	NTNU
AMPD 115-69-5	OECD302C (mod. MITI) -CO2	Activated sludge	30	20			d22: 97%	0,159389	4,3	Laboratory
	OECD306-BOD	Seawater	2	20		4	ND	0,001458	475,3	SINTEF
AEPD 115-70-8	OECD301D-BOD	Activated sludge	2	20		<6		0,002813	246,4	REACH
	OECD301F-DOC	Activated sludge	11	20		8		0,002978	232,7	REACH
	OECD306-BOD	Seawater	2	20		4	ND	0,001458	475,3	SINTEF
TBEA 4620-70-6	OECD306-BOD	Seawater	2	20		7	ND	0,002592	267,4	SINTEF
TBAB 1643-19-2	OECD301D-BOD	Freshwater	2	20		<1		0,000359	1930,7	SINTEF
	OECD301D-BOD	Activated sludge	4	20			d42: 43%	0,013384	51,8	REACH
	OECD306-BOD	Seawater	2	20		<1		0,000359	1930,7	SINTEF
EDA 107-15-3	OECD301D-BOD	Activated sludge	No data	20		95	d16: 88%	0,132516	5,2	REACH
	OECD306-BOD	Seawater	2	20		72	ND	0,045463	15,2	SINTEF
PDA 109-76-2	OECD301A-DOC	Activated sludge	No information	20			d14: 96%	0,229920	3,0	REACH
	OECD306-BOD	Seawater	2	20		72	ND	0,045463	15,2	SINTEF
DMPDA	OECD306-BOD	Seawater	2	20		6	ND	0,002210	313,6	SINTEF

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Name and CAS	Method	Environment	Parameter	Result	UNIT	Project	Laboratory	Reference
Acetic acid 64-19-7	S. costatum-acute	Seawater	EC-50	301	mg/L		Review	ECHA dossier
	D. magna-acute	Freshwater	EC-50	426	mg/L		Review	ECOTOX
	Oncorhynchus kisutch-acute	Freshwater	LC-50	293	mg/L		Review	ECOTOX
Oxalic acid 144-62-7	P. subcapitata-acute	Freshwater	EC-50	19	mg/L		Review	ECHA dossier
	D. magna-acute	Freshwater	EC-50	162	mg/L		Review	ECHA dossier
	Leuciscus idus-acute	Freshwater	LC-50	160	mg/L		Review	ECHA dossier
Bicine 150-25-4	P. subcapitata-acute	Freshwater	EC-50	4930	mg/L	TCM, 2010	SINTEF	Brakstad and da Sil
	P. subcapitata-acute	Freshwater	EC-50	>100	mg/L		Review	ECHA dossier
	Daphnia magna-acute	Freshwater	EC-50	124	mg/L		Review	ECHA dossier
1-hydroxyetane-1,1-diphosphonic acid (HEPD) 2809-21-4	Algae	Freshwater	No relevant data				Review	ECHA dossier
	Daphnia magna-acute	Freshwater	EC-50	527	mg/L		Review	ECHA dossier
	Paleomontes pugios-acute	Saltwater	LC-50	1770	mg/L		Review	ECHA dossier
	Oncorhynchus mykiss-acute	Freshwater	LC-50	195	mg/L		Review	ECHA dossier
	Cyprinodon variegatus-acute	Saltwater	LC-50	2180	mg/L		Review	ECHA dossier
N-(2-hydroxyethyl)glycine (HeGly) 5835-28-9	No data							
Ammonia 7664-41-7	Chlorella vulgaris-acute	Freshwater	EC-50	2700	mg/L		Review	ECHA dossier
	D. magna-acute	Freshwater	EC-50	101	mg/L		Review	ECHA dossier
	Oncorhynchus gorbusch	Freshwater	EC-50	0,068	mg/L		Review	ECHA dossier
Ammonium chloride 12125-02-9	Chlorella vulgaris-acute	Freshwater	EC-50	13000	mg/L		Review	ECHA dossier
	D. magna-acute	Freshwater	EC-50	137	mg/L		Review	ECHA dossier
	Oncorhynchus mykiss-acute	Freshwater	EC-50	43	mg/L		Review	ECHA dossier
Formaldehyde 50-00-0	Desmodesmus suspicatus-acute	Freshwater	EC-50	4,9	mg/L		Review	ECHA dossier
	P. subcapitata-acute	Freshwater	EC-50	4,2	mg/L		Review	ECHA dossier
	Daphnia magna-acute	Freshwater	EC-50	29	mg/L		Review	ECHA dossier
	Daphnia magna -reproduction	Freshwater	NOEC	2,6	mg/L		Review	ECHA dossier
	Pimephales promelas-acute	Freshwater	LC-50	24	mg/L		Review	ECHA dossier
	Morone saxtalis-acute	Seawater	LC-50	6,7	mg/L		Review	ECHA dossier
Acetaldehyde 75-07-0	Nitscheria linearis-acute	Freshwater	LOEC	82	mg/L	TCM, 2010	Review	ECHA dossier
	P. subcapitata-acute	Freshwater	EC-50	36	mg/L		SINTEF	Brakstad and da Sil
	Daphnia magna-acute	Freshwater	EC-50	48	mg/L		Review	ECHA dossier
	Pimephales promelas-acute	Freshwater	LC-50	31	mg/L		Review	ECHA dossier
Ethylene glycol 107-21-1	P. subcapitata-acute	Freshwater	EC-50	3199	mg/L	TCM, 2010	SINTEF	Brakstad and da Sil
	Selenastrum capricornutum-acute	Freshwater	EC-50	6500-13000	mg/L		Review	ECHA dossier
	Daphnia magna-acute	Freshwater	EC-50	>100	mg/L		Review	ECHA dossier
	Pimephales promelas	Freshwater	LC-50	>72850	mg/L		Review	ECHA dossier
Acetone 67-64-1	Microcystis aeruginosa-acute	Freshwater	LOEC	530	mg/L		Review	ECHA dossier
	Prorocentrum minimum-acute	Seawater	NOEC	430	mg/L		Review	ECHA dossier
	Daphnia pulex-acute	Freshwater	EC-50	8800	mg/L		Review	ECHA dossier
	Daphnia magna-chronic	Freshwater	NOEC	2212	mg/L		Review	ECHA dossier
	Artemia salina-acute	Seawater	LC-50	2100	mg/L		Review	ECHA dossier
	Oncorhynchus mykiss-acute	Freshwater	LC-50	5540	mg/L		Review	ECHA dossier
	Alburnus alburnus-acute	Seawater	LC-50	11000	mg/L		Review	ECHA dossier
Acetonitrile 75-05-8	Raphidocelis subcapitata-acute	Freshwater	EC-50	7943	mg/L		Review	ECHA dossier
	Phaeodactylum tricornutum-acute	Seawater	NOEC	400	mg/L		Review	ECHA dossier
	Daphnia magna-acute	Freshwater	EC-50	3600	mg/L		Review	ECHA dossier
	Artemia salina-acute	Seawater	LC-50	400	mg/L		Review	ECHA dossier
	Cyprinus carpio-acute	Freshwater	LC-50	730	mg/L		Review	ECHA dossier
	Pimephales promelas-acute	Freshwater	LC-50	1640	mg/L		Review	ECHA dossier
Methylamine 74-89-5	Green algae-acute	Freshwater	EC-50	47	mg/L	TCM, 2010	Review	ECHA dossier
	P. subcapitata-acute	Freshwater	EC-50	70	mg/L		SINTEF	Brakstad and da Sil
	Daphnia magna-acute	Freshwater	EC-50	163	mg/L		Review	ECHA dossier
	Leuciscus idus-acute	Freshwater	LC-50	970	mg/L		Review	ECHA dossier
	Brachydanio rerio-acute	Freshwater	LC-50	22,9	mM		Review	ECHA dossier
Dimethylamine 124-40-3	Pseudokirchnerella subcapitata-acute	Freshwater	EC-50	9	mg/L	TCM, 2010	Review	ECHA dossier
	P. subcapitata-acute	Freshwater	EC-50	559	mg/L		SINTEF	Brakstad and da Sil
	Chlorella pyrenoidosa-acute	Freshwater	EC-50	30	mg/L		Review	ECHA dossier
	Skeletonema costatum-acute	Seawater	EC-50	28	mg/L	REACT	SINTEF	Eide-Haugmo, 2012
	Daphnia magna-acute	Freshwater	EC-50	89	mg/L		Review	ECHA dossier
	Daphnia magna-acute	Freshwater	EC-50	50	mg/L		Review	ECHA dossier
	Oncorhynchus mykiss-acute	Freshwater	LC-50	118	mg/L		Review	ECHA dossier
Ethylamine 75-04-7	Scenedesmus quadricauda-acute	Freshwater	EC-50	1,6	mg/L	TCM, 2010	Review	ECHA dossier
	P. subcapitata-acute	Freshwater	EC-50	662	mg/L		SINTEF	Brakstad and da Sil
	Scenedesmus quadricauda-acute	Freshwater	EC-50	10	mg/L		Review	ECHA dossier
	Ceriodaphnia dubia-acute	Freshwater	EC-50	7,8	mg/L		Review	ECHA dossier
	Ceriodaphnia dubia-chronic	Freshwater	NOEC	3,2	mg/L		Review	ECHA dossier
	Leuciscus idus-acute	Freshwater	LC-50	168	mg/L		Review	ECHA dossier

Diethylamine 109-89-7	Pseudokirchneriella subcapitata-acute	Freshwater	EC-50	51 mg/L	Review	ECHA dossier
	Pseudokirchneriella subcapitata-chronic	Freshwater	NOEC	34 mg/L	Review	ECHA dossier
	Daphnia magna-acute	Freshwater	EC-50	58 mg/L	Review	ECHA dossier
	Oryzias latipes-acute	Freshwater	LC-50	27 mg/L	Review	ECHA dossier
	Poecilia reticulata	Freshwater	LC-50	130 mg/L	Review	ECHA dossier
Ethyl-methylamine 624-78-2	Pseudokirchneriella subcapitata-acute	Freshwater	EC-50	35 mg/L	Review	ECHA dossier
	Pseudokirchneriella subcapitata-acute	Freshwater	NOEC	17 mg/L	Review	ECHA dossier
	Daphnia magna-acute	Freshwater	EC-50	309 mg/L	Review	ECHA dossier
Propylamine 107-10-8	Daphnia magna-acute	Freshwater	EC-50	71 mg/L	Review	ECHA dossier
	Leuciscus idus-acute	Freshwater	LC-50	46 mg/L	Review	ECHA dossier
2-methyl-2-(methylamino)propane-1-ol 27646-80-6	No data					

Nitromethane 75-52-5	Pseudokirchneriella subcapitata-acute	Freshwater	EC-50		102 mg/L		Review	ECHA dossier
	Pseudokirchneriella subcapitata-acute	Freshwater	NOEC		3,01 mg/L		Review	ECHA dossier
	Daphnia magna-acute	Freshwater	EC-50		103 mg/L		Review	ECHA dossier
	Brachydanio rerio-acute	Freshwater	LC-50		455 mg/L		Review	ECHA dossier
Nitroethane 79-24-3	Pseudokirchneriella subcapitata-acute	Freshwater	EC-50		17 mg/L		Review	ECHA dossier
	Pseudokirchneriella subcapitata-acute	Freshwater	NOEC		7,11 mg/L		Review	ECHA dossier
	Daphnia magna-acute	Freshwater	EC-50		22 mg/L		Review	ECHA dossier
	Brachydanio rerio-acute	Freshwater	LC-50		880 mg/L		Review	ECHA dossier
	Pimephales promelas-acute	Freshwater	LC-50		596 mg/L		Review	ECHA dossier
N-(2-hydroxyethyl)-ethylenediamine (HEED) 111-41-1	Pseudokirchneriella subcapitata-acute	Freshwater	EC-50	>100	mg/L		Review	ECHA dossier
	Pseudokirchneriella subcapitata-acute	Freshwater	EC-10		46 mg/L		Review	ECHA dossier
	Daphnia magna-acute	Freshwater	EC-50	>100	mg/L		Review	ECHA dossier
Formamide 75-12-7	Pseudokirchneriella subcapitata-acute	Freshwater	EC-50	>500	mg/L		Review	ECHA dossier
	Pseudokirchneriella subcapitata-acute	Freshwater	NOEC		125 mg/L		Review	ECHA dossier
	Daphnia magna-acute	Freshwater	EC-50	>500	mg/L		Review	ECHA dossier
	Danio rerio-acute	Freshwater	LC-50		6562 mg/L		Review	ECHA dossier
Acetamide 60-35-5	Scenedesmus quadricauda-acute	Freshwater	EC-50	>10000	mg/L		Review	ECHA dossier
	Daphnia magna-acute	Freshwater	EC-50	>10000	mg/L		Review	ECHA dossier
N-(2-hydroxyethyl)-formamide (HEF) 693-06-1	No data							
N-(2-hydroxyethyl)acetamide (HEA) 142-26-7	Pseudokirchneriella subcapitata-acute	Freshwater	EC-50	>100	mg/L		Review	ECHA dossier
	Pseudokirchneriella subcapitata-acute	Freshwater	NOEC		100 mg/L		Review	ECHA dossier
	Daphnia magna-acute	Freshwater	EC-50	>100	mg/L		Review	ECHA dossier
	Daphnia magna-acute	Freshwater	NOEC		100 mg/L		Review	ECHA dossier
Hydroxyethyl acetamide (HEEAA) 144236-39-5	No data							
N,N'-bis(2-hydroxyethyl) oxamide (BHEOX) 1871-89-2	No data							
Piperazine 110-85-0	Pseudokirchneriella subcapitata-acute	Freshwater	EC50		1271 mg/L	CESAR	SINTEF	CESAR D3.3.3, 2010
	Pseudokirchneriella subcapitata-acute	Freshwater	EC50		472 mg/L	NIVA	Review	Drzyga, O, 2003
	Selenastrum caprocornutum (green algae)-ac	Freshwater	EC50	>1000	mg/L	NIVA	Review	Brooks, 2003
	Skeletonema pseudocostatum-acute	Seawater	EC50		472 mg/L	CESAR	SINTEF	CESAR D3.3.3, 2010
	Skeletonema pseudocostatum-acute	Seawater	EC50		316 mg/L	NIVA	Review	Brooks, 2003
	Daphnia magna-acute	Freshwater	EC50		69 mg/L	CESAR	SINTEF	CESAR D3.3.3, 2010
	Daphnia sp.-acute	Freshwater	EC50		303 mg/L	SOLVIT	SINTEF	SOLVIT D1.3.2 (2012)
	Daphnia sp.-acute	Freshwater	NOEC30		30 mg/L	SOLVIT	SINTEF	SOLVIT D1.3.2 (2012)
	Daphnia sp.-acute	Freshwater	EC50		10-100 mg/L	NIVA	Review	Brooks, 2003
	Cyprino carpio (carp)-acute	Freshwater	LC50		52-159 mg/L	NIVA	Review	Brooks, 2003
	Poecilia reticulata (guppy)-chronic	Freshwater	NOEC		100 mg/L	NIVA	Review	Brooks, 2003
	Kulia sandvicensis (flagtail - bird)-acute	Air	EC50		20 mg/L	NIVA	Review	Brooks, 2003
	4-hydroxyethyl)piperazin-2-one 23936-04-1	No data						
Morpholine 110-91-8	Microtox-acute	Diluent	EC50		32 mg/L	REACT	SINTEF	Eide-Haugmo (2009)
	Selenastrum tricornutum-acute	Freshwater	EC50		28 mg/L			Calamari et al., 1981
	Skeletonema pseudocostatum-acute	Seawater	EC50		9 mg/L	REACT	SINTEF	Eide-Haugmo (2009)
	Daphnia magna-acute	Freshwater	EC50		101 mg/L	REACT	Review	REACT (2007)
	Daphnia magna-acute	Freshwater	EC50		119 mg/L	REACT		Calamari et al., 1981
	Leuciscus idus (carp)-acute	Freshwater	LC50		263 mg/L	REACT	Review	REACT (2007)
	Oncorhynchus mykiss-acute	Freshwater	LC50		380 mg/L	REACT	Review	REACT (2007)
	Salmp gaimeri (fish)-acute	Freshwater	LC50		180 mg/L			Calamari et al., 1981
4-acetomorpholine 1696-20-4	Daphnia magna-acute	Freshwater	EC50		580 mg/L	Read-across 4 -Ethy	Review	ECHA dossier
	Danio rerio-acute	Freshwater	LC-50		6812 mg/L			ECHA dossier
Imidazole 288-32-4	Daphnia magna	Freshwater	EC50		342 mg/L		Review	ECHA dossier
	Leuciscus idus	Freshwater	LC-50		284 mg/L		Review	ECHA dossier
N-(2-hydroxyethyl)imidazole (HEI) 1615-14-1	P. subcapitata-acute	Freshwater	EC-50		30 mg/L	TCM, 2010	SINTEF	Brakstad and da Sil
1-(2-hydroxyethyl)-2-imidazolidone (HEIA) 3699-54-5	Green algae	Freshwater	EC-50		1057 mg/L		Review	ECHA dossier
	P. subcapitata-acute	Freshwater	EC-50	>10000	mg/L	TCM, 2010	SINTEF	Brakstad and da Sil
	P. subcapitata-acute	Freshwater	EC-10	>10000	mg/L	TCM, 2010	SINTEF	Brakstad and da Sil
	Daphnia magna-acute	Freshwater	EC50	>100	mg/L		Review	ECHA dossier
	Oncorhynchus mykiss-acute	Freshwater	LC-50		1004 mg/L		Review	ECHA dossier

Pyrrrole 109-97-7	No data							
1,1'-(1,3-phenylene)bis-1H-pyrrole-2,5-dione 119462-56-5	Pseudokirchneriella subcapitata-acute Daphnia magna-acute Oncorhynchus mykiss	Freshwater Freshwater Freshwater	EC50 EC50 LC-50	67 2,06 0,188	mg/L mg/L mg/L		Review Review Review	ECHA dossier ECHA dossier ECHA dossier
Pyrazine 290-37-9	No data							
Methylpyrazine 109-08-0	No data							
Dimethylpyrazine 123-32-0	No data							
Oxazolidinone 497-25-6	P. subcapitata-acute P. subcapitata-acute	Freshwater Freshwater	EC-50 EC-10 (LOEC)	>10000	mg/L 5544 mg/L	TCM, 2010 TCM, 2010	SINTEF SINTEF	Brakstad and da Silva Brakstad and da Silva
4,4-dimethyloxazolidinone 26654-39-7	P. subcapitata-acute P. subcapitata-acute	Freshwater Freshwater	EC-50 EC-10	>10000	mg/L 3981 mg/L	TCM, 2010 TCM, 2010	SINTEF SINTEF	Brakstad and da Silva Brakstad and da Silva
N-nitrosodiethanolamine (NDELA) 1116-54-7	No data							
Nitrosopiperidine (NPIP) 140-79-4	No data							
Nitrosodiethylamine (NDEA) 55-18-5	S. capricornutum Austropotamobius pallipes-acute Gammarus limnaeus-acute Pimephales promelas-acute	Freshwater Freshwater Freshwater Freshwater	LOEC LC-50 LC-50 LC-50	1 - 10	mg/L 230 mg/L 500 mg/L 775 mg/L	SINTEF NIVA NIVA NIVA	Review Review Review Review	de Silva, 2012 Brooks, 2008 Brooks, 2008 Brooks, 2008
Nitrosodimethylamine (NDMA) 62-75-9	S. capricornutum Gammarus limnaeus-acute Salmo gairdneri-acute Pimephales promelas-acute Oncorhynchus mykiss-chronic	Freshwater Freshwater Freshwater Freshwater Freshwater	LOEC LC-50 LC-50 LC-50 NOEC	1 - 10	mg/L 300 mg/L 1770 mg/L 940 mg/L 200 mg/L	SINTEF NIVA NIVA NIVA SINTEF	Review Review Review Review Review	de Silva, 2012 Brooks, 2008 Brooks, 2008 Brooks, 2008 de Silva, 2012
Nitroso-N-methylethylamine (NMEA) 10595-95-6	No data							
Nitrosomorpholine (NMOR) 59-89-2	Raphidocelis subcapitata	Freshwater	EC-50		84 mg/L		Review	ECOTOX
Nitroso-N-dipropylamine (NDPA) 621-64-7	Lepomis macrochirus	Freshwater	LC-50		5,9 mg/L	NIVA	Review	Brooks, 2008
Nitrosopyrrolidone (NPYR) 930-55-2	No data							
Nitrosopiperazine (NPZ) 5632-47-3	No data							
Dinitrosoperazine (DNPZ) 140-79-4	Poecilia reticulata	Freshwater	LC-50		170 mg/L		Review	ECOTOX
Nitroso(2-hydroxy)glycine (NO-HeGly) 80556-89-4	No data							
Dimethylnitramine (DMNA) 4164-28-7	P. subcapitata-acute Daphnia magna-acute	Freshwater Freshwater	EC-50 EC-50	>2000	mg/L 3042 mg/L	TQPamine5 TQPamine5	SINTEF SINTEF	Dye et al., 2011 Dye et al., 2011
Ethanolnitramine (MEA-NO2) 74386-82-6	P. subcapitata-acute Daphnia magna-acute	Freshwater Freshwater	EC-50 EC-50		2535 mg/L mg/L	TQPamine5 TQPamine5	SINTEF SINTEF	Dye et al., 2011 Dye et al., 2011
Methylnitramine (MNA) 598-57-2	P. subcapitata-acute Daphnia magna-acute	Freshwater Freshwater	EC-50 EC-50		754 mg/L 1426 mg/L	TQPamine5 TQPamine5	SINTEF SINTEF	Dye et al., 2011 Dye et al., 2011
1-nitropiperazine (PZ-NO2) 42499-41-2	P. subcapitata-acute Daphnia magna-acute	Freshwater Freshwater	EC-50 EC-50		430 mg/L 1031 mg/L	TQPamine5 TQPamine5	SINTEF SINTEF	Dye et al., 2011 Dye et al., 2011
1-methyl-2-(nitroamino)-1-propanol (AMP-NO2) 1239666-60-4	P. subcapitata-acute Daphnia magna-acute	Freshwater Freshwater	EC-50 EC-50		871 mg/L 1094 mg/L	TQPamine5 TQPamine5	SINTEF SINTEF	Dye et al., 2011 Dye et al., 2011

Diethylnitramine (DENA)
7119-92-8

No data

Name and CAS	Method	Degradation	Environment	Conc. (mg/L)	Temp (°C)	ThOD	28 days	Other	Rates coefficients	Half-life (d)	Project	Laboratory	Reference
Acetic acid 64-19-7	Study with 14C-acetic acid	Primary (depletion)	Soil	34	20	Not relevant			0,346500	2,0		Review	ECHA dossier
Oxalic acid 144-62-7	BOD	Ultimate	Activated sludge	10	20	No infor		d5: 89%	0,441455	1,6		Review	ECHA dossier
Bicine 150-25-4	OECD301F-manometric	Ultimate	Activated sludge	48	20		94	d14: 77%	0,104977	6,6		Review	ECHA dossier
1-hydroxyetane-1,1-diphosphonic acid (HEPD) 2809-21-4	OECD301D-BOD	Ultimate	Activated sludge	120	20		15		0,005804	119,4		Review	ECHA dossier
N-(2-hydroxyethyl)glycine (HeGly) 5835-28-9	No data												
Ammonia 7664-41-7	Not relevant												
Ammonium chloride 12125-02-9	Not relevant												
Formaldehyde 50-00-0	OECD301A-TOC OECD301C-BOD	Ultimate Ultimate	Activated sludge Activated sludge	20 20	20 20	1,07 1,07	99	d14: 91	0,164470 0,171996	4,2 4,0		Review Review	ECHA dossier ECHA dossier
Acetaldehyde 75-07-0	OECD301C-BOD	Ultimate	Domestic sewage	100	20	1,82		d14: 80	0,114960	6,0		Review	ECHA dossier
Ethylene glycol 107-21-1	OECD301C-BOD OECD301A-DOC	Ultimate Ultimate	Sewage/soil No information	No information No information	20 20			d14: 83% d10: >90%	0,126568 0,230259	5,5 3,0		Review Review	ECHA dossier ECHA dossier
Acetone 67-64-1	OECD301B-CO2 APHA 219-BOD BOD-test	Ultimate Ultimate Ultimate	No information No information saltwater with adapted bact.	No information No information No information	20 20 20		91	d5: 84% d20: 76%	0,085998 0,366516 0,071356	8,1 1,9 9,7		Review Review Review	ECHA dossier ECHA dossier ECHA dossier
Acetonitrile 75-05-8	No information BOD-test				20			d14: 30%	0,025477	27,2		Review Risk report on acetonitrile	ECHA dossier EC, 2010
Methylamine 74-89-5	OECD301C-TOC OECD301F-manometric	Ultimate Ultimate	Activated sludge Activated sludge	100 400	20 20	1,42 3,09	96 55		0,114960 0,028518	6,0 24,3		Review Review	ECHA dossier ECHA dossier
Dimethylamine 124-40-3	OECD301C-TOC OECD306	Ultimate Ultimate	Activated sludge Seawater	100 2	20 20	1,42 1,42	96 77		0,114960 0,052488	6,0 13,2	REACT	Review SINTEF	ECHA dossier Eide-Haugmo, 2012
Ethylamine 75-04-7	OECD301C-BOD	Ultimate	Sludge, soil and water	No information	20		90		0,082235	8,4		Review	ECHA dossier

Name and CAS	Method	Degradation	Environment	Conc. (mg/L)	Temp (°C)	ThOD	28 days	Other	Rates coefficients	Half-life (d)	Project	Laboratory	Reference
Diethylamine 109-89-7	OECD301C-BOD	Ultimate	Activated sludge	No information	20		69		0,041828	16,6		Review	ECHA dossier
	OECD301F-BOD	Ultimate	Activated sludge	No information	20		67		0,039595	17,5		Review	ECHA dossier
Ethyl-methylamine 624-78-2	OECD301D-BOD	Ultimate	No information	No information	20		67		0,039595	17,5		Review	ECHA dossier
Propylamine 107-10-8	OECD310-CO2	Ultimate	Activated sludge	No information	20		78		0,054076	12,8		Review	ECHA dossier
2-methyl-2-(methylamino)propane-1-ol 27646-80-6	No information											Review	ECHA dossier
Nitromethane 75-52-5	OECD301D-BOD	Ultimate	No information	No information	20		<10		0,003763	184,2		Review	ECHA dossier
Nitroethane 79-24-3	OECD301D-BOD	Ultimate	No information	No information	20		<1		0,000359	1930,7		Review	ECHA dossier
	Not standard-CO2	Ultimate	No information	0,05	20?			d5: 24%	0,054887	12,6		Review	ECHA dossier
N-(2-hydroxyethyl)-ethylenediamine (HEED) 111-41-1	No information OECD301C	Ultimate	No information	No information	20		1		0,000359	1930,7		Review Sigma_Aldrich	ECHA dossier HSE sheet
Formamide 75-12-7	OECD301A-DOC	Ultimate	No information	No information	20		>60%		0,032725	21,2		Review	ECHA dossier
Acetamide 60-35-5	OECD301D-BOD		No information	No information	20			d11: 69%	0,106471	6,5		Review	ECHA dossier
N-(2-hydroxyethyl)-formamide (HEF) 693-06-1	No information											Review	ECHA dossier
N-(2-hydroxyethyl)acetamide (HEA) 142-26-7	OECD301D-BOD	Ultimate	Activated sludge	2	20		48		0,023355	29,7		Review	ECHA Dossier
Hydroxyethyl acetamide (HEHEAA) 144236-39-5	No data											Review	ECHA dossier
N,N'-bis(2-hydroxyethyl) oxamide (BHEOX) 1871-89-2	No data												
Piperazine 110-85-0	OECD301F-manometric	Ultimate	Activated sludge	28	20		39		0,017653	39,3		Review	ECHA Dossier
	OECD301D-BOD	Ultimate	Freshwater	2	20		<1		0,000359	1930,7	CESAR	SINTEF	Brakstad et al., 2010
	OECD306-BOD	Ultimate	Seawater	2	20		3		0,001088	637,0	REACT	SINTEF	Eide-Haugmo, 2012
	LC-MS	Primary	Freshwater		20		97		0,125234	5,5	SOLVit	SINTEF	Brakstad et al., 2012
	LC-MS	Primary	Freshwater		10		54,5		0,028123	24,6	SOLVit	SINTEF	Brakstad et al., 2012
LC-MS	Primary	Freshwater		5		11,9		0,004525	153,2	SOLVit	SINTEF	Brakstad et al., 2012	

Name and CAS	Method	Degradation	Environment	Conc. (mg/L)	Temp (°C)	ThOD	28 days	Other	Rates coefficients	Half-life (d)	Project	Laboratory	Reference
4-hydroxyethyl)piperazin-2-one 23936-04-1	No data												
Morpholine 110-91-8	OECD301E-DOC OECD306-BOD	Ultimate Ultimate	Activated sludge Seawater	No information 2	20 20		92 22		0,090205 0,008874	7,7 78,1	REACT	Review SINTEF	ECHA Dossier Eide-Haugmo, 2012
4-acetomorpholine 1696-20-4	OECD302B	Inherent	Activated sludge	No information	20		>60%		0,032725	21,2		Review	ECHA dossier
Imidazole 288-32-4	OECD301A-DOC OECD301C-BOD	Ultimate Ultimate	Activated sludge Activated sludge	No information No information	20 20			d18: 90% 90	0,127921 0,082235	5,4 8,4		Review Review	ECHA dossier ECHA dossier
N-(2-hydroxyethyl)imidazole (HEI) 1615-14-1	No information											Review	ECHA dossier
1-(2-hydroxyethyl)-2-imidazolidone (HEIA) 3699-54-5	ISO7827-DOC OECD302C	Ultimate Inherent	No information No information	No information No information	20 20		1		0,000359 0,065449	1930,7 10,6		Review Review	ECHA dossier ECHA dossier
Pyrrrole 109-97-7	OECD301E-DOC OECD306-BOD	Ultimate Ultimate	Activated sludge Seawater	No information 2	20 20			d9: 95% ND	0,332859 0,067754	2,1 10,2	REACT	Review SINTEF	ECHA Dossier Eide-Haugmo, 2012
1,1'-(1,3-phenylene)bis-1H-pyrrole-2,5-dione 119462-56-5	No information	Ultimate	No information	No information	20		1		0,000359	1930,7		Review	ECHA dossier
Pyrazine 290-37-9	No information											Review	ECHA dossier
Methylpyrazine 109-08-0	No information											Review	ECHA dossier
Dimethylpyrazine 123-32-0	No information OECD306	Ultimate	Seawater	No information	20		22		0,008874	78,1		Review UoStavanger	ECHA dossier
Oxazolidinone 497-25-6	No information											Review	ECHA dossier
4,4-dimethyloxazolidinone 26654-39-7	No information											Review	ECHA dossier
N-nitrosodiethanolamine (NDELA) 1116-54-7	OECD301D-BOD Mod OECD309-LCMS Mod OECD309-LCMS Mod OECD309-LCMS Mod OECD308-LCMS	Ultimate Primary Primary Primary Primary	Lake and river water Lake and river water Lake and river water Lake and river water water/sediment (anaerobic)	2 0,001 0,001 0,001 0,2	20 20 10 5 20	1,55 Not relevant Not relevant Not relevant Not relevant	17	d56: 68% d56: 62 d56: 50 d21: 55%	0,006655 0,020347 0,017278 0,012378 0,038024	104,1 34,1 40,1 56,0 18,2	TCM, 2011 TCM, 2011 TCM, 2011 TCM, 2011 Solvate, 2014	SINTEF SINTEF SINTEF SINTEF SINTEF	Brakstad et al., 2011a Brakstad et al., 2011b Brakstad et al., 2011b Brakstad et al., 2011b Booth et al., 2014
Name and CAS	Method	Degradation	Environment	Conc. (mg/L)	Temp (°C)	ThOD	28 days	Other	Rates coefficients	Half-life (d)	Project	Laboratory	Reference

Nitrosopiperidine (NPIP) 140-79-4	OECD301D-BOD	Ultimate	Lake and river water	2	20	2,38	1		0,000359	1930,7	TCM, 2011	SINTEF	Brakstad et al., 2011a
Name and CAS	Method	Degradation	Environment	Conc. (mg/L)	Temp (°C)	ThOD	28 days	Other	Rates coefficients	Half-life (d)	Project	Laboratory	Reference
Nitrosodiethylamine (NDEA) 55-18-5	OECD301D-BOD	Ultimate	Lake and river water	2	20	2,35	1		0,000359	1930,7	TCM, 2011	SINTEF	Brakstad et al., 2011a
Name and CAS	Method	Degradation	Environment	Conc. (mg/L)	Temp (°C)	ThOD	28 days	Other	Rates coefficients	Half-life (d)	Project	Laboratory	Reference
Nitrosodimethylamine (NDMA) 62-75-9	OECD301D-BOD	Ultimate	Lake and river water	2	20	1,94	1		0,000359	1930,7	TCM, 2011	SINTEF	Brakstad et al., 2011a
	Mod OECD309-LCMS	Primary	Lake and river water	0,005	20	Not relevant		d56: 5%	0,000916	756,6	TCM, 2011	SINTEF	Brakstad et al., 2011b
	Mod OECD308-LCMS	Primary	water/sediment (anaerobic)	0,1	20	Not relevant		d49: 1%	0,000205	3378,7	Solvfate, 2014	SINTEF	Booth et al., 2014
Name and CAS	Method	Degradation	Environment	Conc. (mg/L)	Temp (°C)	ThOD	28 days	Other	Rates coefficients	Half-life (d)	Project	Laboratory	Reference
Nitroso-N-methylethylamine (NMEA) 10595-95-6	OECD301D-BOD	Ultimate	Lake and river water	2	20	2,18	1		0,000359	1930,7	TCM, 2011	SINTEF	Brakstad et al., 2011a
Name and CAS	Method	Degradation	Environment	Conc. (mg/L)	Temp (°C)	ThOD	28 days	Other	Rates coefficients	Half-life (d)	Project	Laboratory	Reference
Nitrosomorpholine (NMOR) 59-89-2	OECD301D-BOD	Ultimate	Lake and river water	2	20	1,79	1		0,000359	1930,7	TCM, 2011	SINTEF	Brakstad et al., 2011a
Name and CAS	Method	Degradation	Environment	Conc. (mg/L)	Temp (°C)	ThOD	28 days	Other	Rates coefficients	Half-life (d)	Project	Laboratory	Reference
Nitroso-N-dipropylamine (NDPA) 621-64-7	OECD301D-BOD	Ultimate	Lake and river water	2	20	2,58	1		0,000359	1930,7	TCM, 2011	SINTEF	Brakstad et al., 2011a
Name and CAS	Method	Degradation	Environment	Conc. (mg/L)	Temp (°C)	ThOD	28 days	Other	Rates coefficients	Half-life (d)	Project	Laboratory	Reference
Nitrosopyrrolidone (NPYR) 930-55-2	OECD301D-BOD	Ultimate	Lake and river water	2	20	2,24	1		0,000359	1930,7	TCM, 2011	SINTEF	Brakstad et al., 2011a
Name and CAS	Method	Degradation	Environment	Conc. (mg/L)	Temp (°C)	ThOD	28 days	Other	Rates coefficients	Half-life (d)	Project	Laboratory	Reference
Nitrosopiperazine (NPZ) 5632-47-3	OECD301D-BOD	Ultimate	Lake and river water	2	20	2,22	1		0,000359	1930,7	TCM, 2011	SINTEF	Brakstad et al., 2011a
	Mod OECD309-LCMS	Primary	Lake and river water	0,01	20	Not relevant		d56: 1%			TCM, 2011	SINTEF	Brakstad et al., 2011b
Name and CAS	Method	Degradation	Environment	Conc. (mg/L)	Temp (°C)	ThOD	28 days	Other	Rates coefficients	Half-life (d)	Project	Laboratory	Reference
Dinitrosoperazine (DNPZ) 140-79-4	OECD301D-BOD	Ultimate	Lake and river water	2	20	1,78	1		0,000359	1930,7	TCM, 2011	SINTEF	Brakstad et al., 2011a
Name and CAS	Method	Degradation	Environment	Conc. (mg/L)	Temp (°C)	ThOD	28 days	Other	Rates coefficients	Half-life (d)	Project	Laboratory	Reference
Nitroso(2-hydroxy)glycine (NO-HeGly) 80556-89-4	No data												
Name and CAS	Method	Degradation	Environment	Conc. (mg/L)	Temp (°C)	ThOD	28 days	Other	Rates coefficients	Half-life (d)	Project	Laboratory	Reference
Dimethylnitramine (DMNA) 4164-28-7	Mod OECD309-LCMS	Primary	Lake and river water	0,002	20	Not relevant			0,01829	37,9	TCM, 2014	SINTEF	Brakstad et al., 2014
	OECD301D-BOD	Ultimate	Lake and river water	2	20	1,42	3,4		0,001235	560,9	TQPAmine5, 2011	SINTEF	Dye et al., 2011
	Mod OECD308-LCMS	Primary	water/sediment (anaerobic)	0,1	20	Not relevant		d49: 18%	0,004050	171,1	Solvfate, 2014	SINTEF	Booth et al., 2014
Name and CAS	Method	Degradation	Environment	Conc. (mg/L)	Temp (°C)	ThOD	28 days	Other	Rates coefficients	Half-life (d)	Project	Laboratory	Reference
Ethanolnitramine (MEA-NO2) 74386-82-6	Mod OECD309-LCMS	Primary	Lake and river water	0,02	20	Not relevant			0,08319	28,7	TCM, 2014	SINTEF	Brakstad et al., 2014
	OECD301D-BOD	Ultimate	Lake and river water	2	20	1,06	33		0,014303	48,5	TQPAmine5, 2011	SINTEF	Dye et al., 2011
	Mod OECD308-LCMS	Primary	water/sediment (anaerobic)	0,1	20	Not relevant		d21: 85%	0,090339	7,7	Solvfate, 2014	SINTEF	Booth et al., 2014
Name and CAS	Method	Degradation	Environment	Conc. (mg/L)	Temp (°C)	ThOD	28 days	Other	Rates coefficients	Half-life (d)	Project	Laboratory	Reference
Methylnitramine (MNA) 598-57-2	Mod OECD309-LCMS	Primary	Lake and river water	0,05	20	Not relevant	1		0,000359	1930,7	TCM, 2014	SINTEF	Brakstad et al., 2014
	OECD301D-BOD	Ultimate	Lake and river water	2	20	1,05	34		0,014840	46,7			
Name and CAS	Method	Degradation	Environment	Conc. (mg/L)	Temp (°C)	ThOD	28 days	Other	Rates coefficients	Half-life (d)	Project	Laboratory	Reference
1-nitropiperazine (PZ-NO2) 42499-41-2	Mod OECD309-LCMS	Primary	Lake and river water	0,02	20	Not relevant	1		0,000359	1930,7	TCM, 2014	SINTEF	Brakstad et al., 2014
	OECD301D-BOD	Ultimate	Lake and river water	2	20	1,5	3		0,001088	637,0	TQPAmine5, 2011	SINTEF	Dye et al., 2011
Name and CAS	Method	Degradation	Environment	Conc. (mg/L)	Temp (°C)	ThOD	28 days	Other	Rates coefficients	Half-life (d)	Project	Laboratory	Reference
1-methyl-2-(nitroamino)-1-propanol (AMP-NO2) 1239666-60-4	Mod OECD309-LCMS	Primary	Lake and river water	0,02	20	Not relevant			0,05256	38,7	TCM, 2014	SINTEF	Brakstad et al., 2014
	OECD301D-BOD	Ultimate	Lake and river water	2	20	1,55	20		0,007969	87,0	TQPAmine5, 2011	SINTEF	Dye et al., 2011

Name and CAS	Method	Degradation	Environment	Conc. (mg/L)	Temp (°C)	ThOD	28 days	Other	Rates coefficients	Half-life (d)	Project	Laboratory	Reference
Diethylnitramine (DENA) 7119-92-8	Mod OECD309-LCMS	Primary	Lake and river water	0,05	20	Not relevant	1		0,000359	1930,7	TCM, 2014	SINTEF	Brakstad et al., 2014

Name and CAS	Method	Environment	Conc. (mg/L)	Temp (°C)	ThOD	28 days	Other	Rates coefficients	Half-life (d)	Laboratory
MEA 141-43-5	OECD301D-BOD	Freshwater	2	20		64	ND	0,036488	19,0	SINTEF
	OECD306-BOD	Seawater	2	20		68	ND	0,040694	17,0	SINTEF
	OECD301B-CO2	Activated sludge	19	20		83	ND	0,063284	11,0	REVIEW
	OECD301B-CO2	Activated sludge	20	20		62	ND	0,034557	20,1	Review
	OECD301D-BOD	Freshwater	2	20		78	ND	0,054076	12,8	NTNU
AP 156-87-6	OECD 301C (MITI)-BOD	Mix (sludge, water, etc.)	No information	20		86	ND	0,070218	9,9	REACH
	OECD306-BOD	Seawater	2	20		3	ND	0,001088	637,0	SINTEF
AB 13325-10-5	OECD306-BOD	Seawater	2	20		69	ND	0,041828	16,6	SINTEF
MIPA 78-96-6	OECD301F-manometry	Activated sludge	100	20			d3: 60%	0,305430	2,3	REACH
	OECD306-BOD	Seawater	2	20		58	ND	0,030982	22,4	SINTEF
DGA 929-06-6	OECD301B-DOC	Activated sludge	No information	20		84		0,065449	10,6	REACH
	OECD306-BOD	Seawater	2	20		<1	ND	0,000359	1930,7	SINTEF
MMEA 109-83-1	OECD301A-DOC	Activated sludge	20 mg/L DOC	20			d21: 93%	0,126631	5,5	REACH
	OECD306-BOD	Seawater	2	20		77	ND	0,052488	13,2	SINTEF
EAE 110-73-6	OECD301D-CO2	Activated sludge	10 and 20	20		62		0,034557	20,1	REACH
	OECD306-BOD	Seawater	2	20		70	ND	0,042999	16,1	SINTEF
DEA 111-42-2	OECD301F-manometric	Activated sludge	No data	20		93		0,094974	7,3	REACH
	OECD306-BOD	Seawater	2	20		63	ND	0,035509	19,5	SINTEF
	OECD301D-BOD	Freshwater	2	20		83,2		0,063707	10,9	NTNU
DIPA 110-97-4	OECD301F-manometric	Activated sludge	No data	20		94		0,100479	6,9	REACH
	OECD306-BOD	Seawater	2	20		<1	ND	0,000359	1930,7	SINTEF
AEAA 111-41-1	OECD301F-manometric	Activated sludge	No data	20		45		0,021351	32,5	REACH
	OECD306-BOD	Seawater	2	20		3	ND	0,001088	637,0	SINTEF
BHE 4439-20-7	OECD306-BOD	Seawater	2	20		30	ND	0,012738	54,4	SINTEF
DMMEA 108-01-0	OECD301C-BOD	Mix activ. sludge, water, etc.	100	20			d14: 61%	0,083656	8,3	REACH
	OECD301D-BOD	Freshwater	2	20		86,8		0,072320	9,6	SINTEF
	OECD306-BOD	Seawater	2	20		94		0,100479	6,9	SINTEF
MDEA 105-59-9	OECD301A-DOC	Activated sludge	No data	20			d18: 96%	0,178826	3,9	REACH
	OECD306-BOD	Seawater	2	20		<1	ND	0,000359	1930,7	SINTEF
	OECD301D-BOD	Freshwater	2	20		77,3		0,052957	13,1	NTNU
DEEA 100-37-8	OECD301D-BOD	Activated sludge	No information	20			d10: 82%	0,171480	4,0	REACH
	OECD301D-BOD	Freshwater	2	20		79,2		0,056079	12,4	SINTEF
	OECD306-BOD	Seawater	2	20		2		0,000722	960,5	SINTEF
	OECD306-BOD	Seawater	2	20		<1		0,000359	1930,7	SINTEF
TEA 102-71-6	No information	Activated sludge	168	No information		No information			0,24	REACH
	OECD306-BOD	Seawater	2	20		20	ND	0,007969	87,0	SINTEF
DMPA 3179-63-3	OECD301A-DOC	Activated sludge	No information	20		99		0,164470	4,2	REACH
	OECD306-BOD	Seawater	2	20		16	ND	0,006227	111,3	SINTEF
1DMA2P 108-16-7	OECD301A-DOC	Activated sludge	No information	20		90		0,082235	8,4	REACH
	OECD306-BOD	Seawater	2	20		5	ND	0,001832	378,3	SINTEF
AMP 124-68-5	OECD301F-manometric	Activated sludge	11	20		89		0,078831	8,8	REACH
	OECD301D-BOD	Freshwater	2	20		25,7	ND	0,010609	65,3	SINTEF
	OECD306	Closed bottle (BOD)	2	20		<1	ND	0,000359	1930,7	SINTEF
	Primary deg/LC-MS	Freshwater	0,01	20	Not relevant	97	ND	0,077	9,0	SINTEF
	Primary deg/LC-MS	Freshwater	0,01	10	Not relevant	97	ND	0,077	9,0	SINTEF
	Primary deg/LC-MS	Freshwater	0,01	5	Not relevant	4,3	d56: 97	0,0218	31,8	SINTEF
	OECD301D-BOD	Freshwater	2	20		83,3	ND	0,063920	10,8	NTNU
AMPD 115-69-5	OECD302C (mod. MITI) -CO2	Activated sludge	30	20			d22: 97%	0,159389	4,3	Laboratory
	OECD306-BOD	Seawater	2	20		4	ND	0,001458	475,3	SINTEF
AEPD 115-70-8	OECD301D-BOD	Activated sludge	2	20		<6		0,002813	246,4	REACH
	OECD301F-DOC	Activated sludge	11	20		8		0,002978	232,7	REACH
	OECD306-BOD	Seawater	2	20		4	ND	0,001458	475,3	SINTEF
TBEA 4620-70-6	OECD306-BOD	Seawater	2	20		7	ND	0,002592	267,4	SINTEF
TBAB 1643-19-2	OECD301D-BOD	Freshwater	2	20		<1		0,000359	1930,7	SINTEF
	OECD301D-BOD	Activated sludge	4	20			d42: 43%	0,013384	51,8	REACH
	OECD306-BOD	Seawater	2	20		<1		0,000359	1930,7	SINTEF
EDA 107-15-3	OECD301D-BOD	Activated sludge	No data	20		95	d16: 88%	0,132516	5,2	REACH
	OECD306-BOD	Seawater	2	20		72	ND	0,045463	15,2	SINTEF
PDA 109-76-2	OECD301A-DOC	Activated sludge	No information	20			d14: 96%	0,229920	3,0	REACH
	OECD306-BOD	Seawater	2	20		72	ND	0,045463	15,2	SINTEF
DMPDA	OECD306-BOD	Seawater	2	20		6	ND	0,002210	313,6	SINTEF

Reference

Cesar D3.3.3 (2010)
Eide-Haugmo, 2012
SOLVit D1.4.1 (2009)
SOLVit D1.4.1 (2009)
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Reference

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Reference

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Eide-Haugmo, 2012

Name and CAS	Method	Environment	Parameter	Result	UNIT	Project	Laboratory	Reference
Acetic acid 64-19-7	S. costatum-acute	Seawater	EC-50	301	mg/L		Review	ECHA dossier
	D. magna-acute	Freshwater	EC-50	426	mg/L		Review	ECOTOX
	Oncorhynchus kisutch-acute	Freshwater	LC-50	293	mg/L		Review	ECOTOX
Oxalic acid 144-62-7	P. subcapitata-acute	Freshwater	EC-50	19	mg/L		Review	ECHA dossier
	D. magna-acute	Freshwater	EC-50	162	mg/L		Review	ECHA dossier
	Leuciscus idus-acute	Freshwater	LC-50	160	mg/L		Review	ECHA dossier
Bicine 150-25-4	P. subcapitata-acute	Freshwater	EC-50	4930	mg/L	TCM, 2010	SINTEF	Brakstad and da Sil
	P. subcapitata-acute	Freshwater	EC-50	>100	mg/L		Review	ECHA dossier
	Daphnia magna-acute	Freshwater	EC-50	124	mg/L		Review	ECHA dossier
1-hydroxyetane-1,1-diphosphonic acid (HEPD) 2809-21-4	Algae	Freshwater	No relevant data				Review	ECHA dossier
	Daphnia magna-acute	Freshwater	EC-50	527	mg/L		Review	ECHA dossier
	Paleomontes pugios-acute	Saltwater	LC-50	1770	mg/L		Review	ECHA dossier
	Oncorhynchus mykiss-acute	Freshwater	LC-50	195	mg/L		Review	ECHA dossier
	Cyprinodon variegatus-acute	Saltwater	LC-50	2180	mg/L		Review	ECHA dossier
N-(2-hydroxyethyl)glycine (HeGly) 5835-28-9	No data							
Ammonia 7664-41-7	Chlorella vulgaris-acute	Freshwater	EC-50	2700	mg/L		Review	ECHA dossier
	D. magna-acute	Freshwater	EC-50	101	mg/L		Review	ECHA dossier
	Oncorhynchus gorbusch	Freshwater	EC-50	0,068	mg/L		Review	ECHA dossier
Ammonium chloride 12125-02-9	Chlorella vulgaris-acute	Freshwater	EC-50	13000	mg/L		Review	ECHA dossier
	D. magna-acute	Freshwater	EC-50	137	mg/L		Review	ECHA dossier
	Oncorhynchus mykiss-acute	Freshwater	EC-50	43	mg/L		Review	ECHA dossier
Formaldehyde 50-00-0	Desmodesmus suspicatus-acute	Freshwater	EC-50	4,9	mg/L		Review	ECHA dossier
	P. subcapitata-acute	Freshwater	EC-50	4,2	mg/L		Review	ECHA dossier
	Daphnia magna-acute	Freshwater	EC-50	29	mg/L		Review	ECHA dossier
	Daphnia magna -reproduction	Freshwater	NOEC	2,6	mg/L		Review	ECHA dossier
	Pimephales promelas-acute	Freshwater	LC-50	24	mg/L		Review	ECHA dossier
	Morone saxtalis-acute	Seawater	LC-50	6,7	mg/L		Review	ECHA dossier
Acetaldehyde 75-07-0	Nitscheria linearis-acute	Freshwater	LOEC	82	mg/L	TCM, 2010	Review	ECHA dossier
	P. subcapitata-acute	Freshwater	EC-50	36	mg/L		SINTEF	Brakstad and da Sil
	Daphnia magna-acute	Freshwater	EC-50	48	mg/L		Review	ECHA dossier
	Pimephales promelas-acute	Freshwater	LC-50	31	mg/L		Review	ECHA dossier
Ethylene glycol 107-21-1	P. subcapitata-acute	Freshwater	EC-50	3199	mg/L	TCM, 2010	SINTEF	Brakstad and da Sil
	Selenastrum capricornutum-acute	Freshwater	EC-50	6500-13000	mg/L		Review	ECHA dossier
	Daphnia magna-acute	Freshwater	EC-50	>100	mg/L		Review	ECHA dossier
	Pimephales promelas	Freshwater	LC-50	>72850	mg/L		Review	ECHA dossier
Acetone 67-64-1	Microcystis aeruginosa-acute	Freshwater	LOEC	530	mg/L		Review	ECHA dossier
	Prorocentrum minimum-acute	Seawater	NOEC	430	mg/L		Review	ECHA dossier
	Daphnia pulex-acute	Freshwater	EC-50	8800	mg/L		Review	ECHA dossier
	Daphnia magna-chronic	Freshwater	NOEC	2212	mg/L		Review	ECHA dossier
	Artemia salina-acute	Seawater	LC-50	2100	mg/L		Review	ECHA dossier
	Oncorhynchus mykiss-acute	Freshwater	LC-50	5540	mg/L		Review	ECHA dossier
	Alburnus alburnus-acute	Seawater	LC-50	11000	mg/L		Review	ECHA dossier
Acetonitrile 75-05-8	Raphidocelis subcapitata-acute	Freshwater	EC-50	7943	mg/L		Review	ECHA dossier
	Phaeodactylum tricornutum-acute	Seawater	NOEC	400	mg/L		Review	ECHA dossier
	Daphnia magna-acute	Freshwater	EC-50	3600	mg/L		Review	ECHA dossier
	Artemia salina-acute	Seawater	LC-50	400	mg/L		Review	ECHA dossier
	Cyprinus carpio-acute	Freshwater	LC-50	730	mg/L		Review	ECHA dossier
	Pimephales promelas-acute	Freshwater	LC-50	1640	mg/L		Review	ECHA dossier
Methylamine 74-89-5	Green algae-acute	Freshwater	EC-50	47	mg/L	TCM, 2010	Review	ECHA dossier
	P. subcapitata-acute	Freshwater	EC-50	70	mg/L		SINTEF	Brakstad and da Sil
	Daphnia magna-acute	Freshwater	EC-50	163	mg/L		Review	ECHA dossier
	Leuciscus idus-acute	Freshwater	LC-50	970	mg/L		Review	ECHA dossier
	Brachydanio rerio-acute	Freshwater	LC-50	22,9	mM		Review	ECHA dossier
Dimethylamine 124-40-3	Pseudokirchnerella subcapitata-acute	Freshwater	EC-50	9	mg/L	TCM, 2010	Review	ECHA dossier
	P. subcapitata-acute	Freshwater	EC-50	559	mg/L		SINTEF	Brakstad and da Sil
	Chlorella pyrenoidosa-acute	Freshwater	EC-50	30	mg/L		Review	ECHA dossier
	Skeletonema costatum-acute	Seawater	EC-50	28	mg/L	REACT	SINTEF	Eide-Haugmo, 2012
	Daphnia magna-acute	Freshwater	EC-50	89	mg/L		Review	ECHA dossier
	Daphnia magna-acute	Freshwater	EC-50	50	mg/L		Review	ECHA dossier
	Oncorhynchus mykiss-acute	Freshwater	LC-50	118	mg/L		Review	ECHA dossier
Ethylamine 75-04-7	Scenedesmus quadricauda-acute	Freshwater	EC-50	1,6	mg/L	TCM, 2010	Review	ECHA dossier
	P. subcapitata-acute	Freshwater	EC-50	662	mg/L		SINTEF	Brakstad and da Sil
	Scenedesmus quadricauda-acute	Freshwater	EC-50	10	mg/L		Review	ECHA dossier
	Ceriodaphnia dubia-acute	Freshwater	EC-50	7,8	mg/L		Review	ECHA dossier
	Ceriodaphnia dubia-chronic	Freshwater	NOEC	3,2	mg/L		Review	ECHA dossier
	Leuciscus idus-acute	Freshwater	LC-50	168	mg/L		Review	ECHA dossier

Diethylamine 109-89-7	Pseudokirchneriella subcapitata-acute	Freshwater	EC-50	51 mg/L	Review	ECHA dossier
	Pseudokirchneriella subcapitata-chronic	Freshwater	NOEC	34 mg/L	Review	ECHA dossier
	Daphnia magna-acute	Freshwater	EC-50	58 mg/L	Review	ECHA dossier
	Oryzias latipes-acute	Freshwater	LC-50	27 mg/L	Review	ECHA dossier
	Poecilia reticulata	Freshwater	LC-50	130 mg/L	Review	ECHA dossier
Ethyl-methylamine 624-78-2	Pseudokirchneriella subcapitata-acute	Freshwater	EC-50	35 mg/L	Review	ECHA dossier
	Pseudokirchneriella subcapitata-acute	Freshwater	NOEC	17 mg/L	Review	ECHA dossier
	Daphnia magna-acute	Freshwater	EC-50	309 mg/L	Review	ECHA dossier
Propylamine 107-10-8	Daphnia magna-acute	Freshwater	EC-50	71 mg/L	Review	ECHA dossier
	Leuciscus idus-acute	Freshwater	LC-50	46 mg/L	Review	ECHA dossier
2-methyl-2-(methylamino)propane-1-ol 27646-80-6	No data					

Nitromethane 75-52-5	Pseudokirchneriella subcapitata-acute	Freshwater	EC-50		102 mg/L		Review	ECHA dossier
	Pseudokirchneriella subcapitata-acute	Freshwater	NOEC		3,01 mg/L		Review	ECHA dossier
	Daphnia magna-acute	Freshwater	EC-50		103 mg/L		Review	ECHA dossier
	Brachydanio rerio-acute	Freshwater	LC-50		455 mg/L		Review	ECHA dossier
Nitroethane 79-24-3	Pseudokirchneriella subcapitata-acute	Freshwater	EC-50		17 mg/L		Review	ECHA dossier
	Pseudokirchneriella subcapitata-acute	Freshwater	NOEC		7,11 mg/L		Review	ECHA dossier
	Daphnia magna-acute	Freshwater	EC-50		22 mg/L		Review	ECHA dossier
	Brachydanio rerio-acute	Freshwater	LC-50		880 mg/L		Review	ECHA dossier
	Pimephales promelas-acute	Freshwater	LC-50		596 mg/L		Review	ECHA dossier
N-(2-hydroxyethyl)-ethylenediamine (HEED) 111-41-1	Pseudokirchneriella subcapitata-acute	Freshwater	EC-50	>100	mg/L		Review	ECHA dossier
	Pseudokirchneriella subcapitata-acute	Freshwater	EC-10		46 mg/L		Review	ECHA dossier
	Daphnia magna-acute	Freshwater	EC-50	>100	mg/L		Review	ECHA dossier
Formamide 75-12-7	Pseudokirchneriella subcapitata-acute	Freshwater	EC-50	>500	mg/L		Review	ECHA dossier
	Pseudokirchneriella subcapitata-acute	Freshwater	NOEC		125 mg/L		Review	ECHA dossier
	Daphnia magna-acute	Freshwater	EC-50	>500	mg/L		Review	ECHA dossier
	Danio rerio-acute	Freshwater	LC-50		6562 mg/L		Review	ECHA dossier
Acetamide 60-35-5	Scenedesmus quadricauda-acute	Freshwater	EC-50	>10000	mg/L		Review	ECHA dossier
	Daphnia magna-acute	Freshwater	EC-50	>10000	mg/L		Review	ECHA dossier
N-(2-hydroxyethyl)-formamide (HEF) 693-06-1	No data							
N-(2-hydroxyethyl)acetamide (HEA) 142-26-7	Pseudokirchneriella subcapitata-acute	Freshwater	EC-50	>100	mg/L		Review	ECHA dossier
	Pseudokirchneriella subcapitata-acute	Freshwater	NOEC		100 mg/L		Review	ECHA dossier
	Daphnia magna-acute	Freshwater	EC-50	>100	mg/L		Review	ECHA dossier
	Daphnia magna-acute	Freshwater	NOEC		100 mg/L		Review	ECHA dossier
Hydroxyethyl acetamide (HEEAA) 144236-39-5	No data							
N,N'-bis(2-hydroxyethyl) oxamide (BHEOX) 1871-89-2	No data							
Piperazine 110-85-0	Pseudokirchneriella subcapitata-acute	Freshwater	EC50		1271 mg/L	CESAR	SINTEF	CESAR D3.3.3, 2010
	Pseudokirchneriella subcapitata-acute	Freshwater	EC50		472 mg/L	NIVA	Review	Drzyga, O, 2003
	Selenastrum caprocornutum (green algae)-ac	Freshwater	EC50	>1000	mg/L	NIVA	Review	Brooks, 2003
	Skeletonema pseudocostatum-acute	Seawater	EC50		472 mg/L	CESAR	SINTEF	CESAR D3.3.3, 2010
	Skeletonema pseudocostatum-acute	Seawater	EC50		316 mg/L	NIVA	Review	Brooks, 2003
	Daphnia magna-acute	Freshwater	EC50		69 mg/L	CESAR	SINTEF	CESAR D3.3.3, 2010
	Daphnia sp.-acute	Freshwater	EC50		303 mg/L	SOLVIT	SINTEF	SOLVIT D1.3.2 (2012)
	Daphnia sp.-acute	Freshwater	NOEC30		30 mg/L	SOLVIT	SINTEF	SOLVIT D1.3.2 (2012)
	Daphnia sp.-acute	Freshwater	EC50		10-100 mg/L	NIVA	Review	Brooks, 2003
	Cyprino carpio (carp)-acute	Freshwater	LC50		52-159 mg/L	NIVA	Review	Brooks, 2003
	Poecilia reticulata (guppy)-chronic	Freshwater	NOEC		100 mg/L	NIVA	Review	Brooks, 2003
	Kulia sandvicensis (flagtail - bird)-acute	Air	EC50		20 mg/L	NIVA	Review	Brooks, 2003
	4-hydroxyethyl)piperazin-2-one 23936-04-1	No data						
Morpholine 110-91-8	Microtox-acute	Diluent	EC50		32 mg/L	REACT	SINTEF	Eide-Haugmo (2009)
	Selenastrum tricornutum-acute	Freshwater	EC50		28 mg/L			Calamari et al., 1981
	Skeletonema pseudocostatum-acute	Seawater	EC50		9 mg/L	REACT	SINTEF	Eide-Haugmo (2009)
	Daphnia magna-acute	Freshwater	EC50		101 mg/L	REACT	Review	REACT (2007)
	Daphnia magna-acute	Freshwater	EC50		119 mg/L	REACT		Calamari et al., 1981
	Leuciscus idus (carp)-acute	Freshwater	LC50		263 mg/L	REACT	Review	REACT (2007)
	Oncorhynchus mykiss-acute	Freshwater	LC50		380 mg/L	REACT	Review	REACT (2007)
	Salmp gairmeri (fish)-acute	Freshwater	LC50		180 mg/L			Calamari et al., 1981
4-acetomorpholine 1696-20-4	Daphnia magna-acute	Freshwater	EC50		580 mg/L	Read-across 4 -Ethy	Review	ECHA dossier
	Danio rerio-acute	Freshwater	LC-50		6812 mg/L			ECHA dossier
Imidazole 288-32-4	Daphnia magna	Freshwater	EC50		342 mg/L		Review	ECHA dossier
	Leuciscus idus	Freshwater	LC-50		284 mg/L		Review	ECHA dossier
N-(2-hydroxyethyl)imidazole (HEI) 1615-14-1	P. subcapitata-acute	Freshwater	EC-50		30 mg/L	TCM, 2010	SINTEF	Brakstad and da Sil
1-(2-hydroxyethyl)-2-imidazolidone (HEIA) 3699-54-5	Green algae	Freshwater	EC-50		1057 mg/L		Review	ECHA dossier
	P. subcapitata-acute	Freshwater	EC-50	>10000	mg/L	TCM, 2010	SINTEF	Brakstad and da Sil
	P. subcapitata-acute	Freshwater	EC-10	>10000	mg/L	TCM, 2010	SINTEF	Brakstad and da Sil
	Daphnia magna-acute	Freshwater	EC50	>100	mg/L		Review	ECHA dossier
	Oncorhynchus mykiss-acute	Freshwater	LC-50		1004 mg/L		Review	ECHA dossier

Pyrrrole 109-97-7	No data							
1,1'-(1,3-phenylene)bis-1H-pyrrole-2,5-dione 119462-56-5	Pseudokirchneriella subcapitata-acute Daphnia magna-acute Oncorhynchus mykiss	Freshwater Freshwater Freshwater	EC50 EC50 LC-50	67 2,06 0,188	mg/L mg/L mg/L		Review Review Review	ECHA dossier ECHA dossier ECHA dossier
Pyrazine 290-37-9	No data							
Methylpyrazine 109-08-0	No data							
Dimethylpyrazine 123-32-0	No data							
Oxazolidinone 497-25-6	P. subcapitata-acute P. subcapitata-acute	Freshwater Freshwater	EC-50 EC-10 (LOEC)	>10000	mg/L 5544 mg/L	TCM, 2010 TCM, 2010	SINTEF SINTEF	Brakstad and da Silva Brakstad and da Silva
4,4-dimethyloxazolidinone 26654-39-7	P. subcapitata-acute P. subcapitata-acute	Freshwater Freshwater	EC-50 EC-10	>10000	mg/L 3981 mg/L	TCM, 2010 TCM, 2010	SINTEF SINTEF	Brakstad and da Silva Brakstad and da Silva
N-nitrosodiethanolamine (NDELA) 1116-54-7	No data							
Nitrosopiperidine (NPIP) 140-79-4	No data							
Nitrosodiethylamine (NDEA) 55-18-5	S. capricornutum Austropotamobius pallipes-acute Gammarus limnaeus-acute Pimephales promelas-acute	Freshwater Freshwater Freshwater Freshwater	LOEC LC-50 LC-50 LC-50	1 - 10	mg/L 230 mg/L 500 mg/L 775 mg/L	SINTEF NIVA NIVA NIVA	Review Review Review Review	de Silva, 2012 Brooks, 2008 Brooks, 2008 Brooks, 2008
Nitrosodimethylamine (NDMA) 62-75-9	S. capricornutum Gammarus limnaeus-acute Salmo gairdneri-acute Pimephales promelas-acute Oncorhynchus mykiss-chronic	Freshwater Freshwater Freshwater Freshwater Freshwater	LOEC LC-50 LC-50 LC-50 NOEC	1 - 10	mg/L 300 mg/L 1770 mg/L 940 mg/L 200 mg/L	SINTEF NIVA NIVA NIVA SINTEF	Review Review Review Review Review	de Silva, 2012 Brooks, 2008 Brooks, 2008 Brooks, 2008 de Silva, 2012
Nitroso-N-methylethylamine (NMEA) 10595-95-6	No data							
Nitrosomorpholine (NMOR) 59-89-2	Raphidocelis subcapitata	Freshwater	EC-50		84 mg/L		Review	ECOTOX
Nitroso-N-dipropylamine (NDPA) 621-64-7	Lepomis macrochirus	Freshwater	LC-50		5,9 mg/L	NIVA	Review	Brooks, 2008
Nitrosopyrrolidone (NPYR) 930-55-2	No data							
Nitrosopiperazine (NPZ) 5632-47-3	No data							
Dinitrosoperazine (DNPZ) 140-79-4	Poecilia reticulata	Freshwater	LC-50		170 mg/L		Review	ECOTOC
Nitroso(2-hydroxy)glycine (NO-HeGly) 80556-89-4	No data							
Dimethylnitramine (DMNA) 4164-28-7	P. subcapitata-acute Daphnia magna-acute	Freshwater Freshwater	EC-50 EC-50	>2000	mg/L 3042 mg/L	TQPamine5 TQPamine5	SINTEF SINTEF	Dye et al., 2011 Dye et al., 2011
Ethanolnitramine (MEA-NO2) 74386-82-6	P. subcapitata-acute Daphnia magna-acute	Freshwater Freshwater	EC-50 EC-50		2535 mg/L mg/L	TQPamine5 TQPamine5	SINTEF SINTEF	Dye et al., 2011 Dye et al., 2011
Methylnitramine (MNA) 598-57-2	P. subcapitata-acute Daphnia magna-acute	Freshwater Freshwater	EC-50 EC-50		754 mg/L 1426 mg/L	TQPamine5 TQPamine5	SINTEF SINTEF	Dye et al., 2011 Dye et al., 2011
1-nitropiperazine (PZ-NO2) 42499-41-2	P. subcapitata-acute Daphnia magna-acute	Freshwater Freshwater	EC-50 EC-50		430 mg/L 1031 mg/L	TQPamine5 TQPamine5	SINTEF SINTEF	Dye et al., 2011 Dye et al., 2011
1-methyl-2-(nitroamino)-1-propanol (AMP-NO2) 1239666-60-4	P. subcapitata-acute Daphnia magna-acute	Freshwater Freshwater	EC-50 EC-50		871 mg/L 1094 mg/L	TQPamine5 TQPamine5	SINTEF SINTEF	Dye et al., 2011 Dye et al., 2011

Diethylnitramine (DENA)
7119-92-8

No data

Name and CAS	Method	Degradation	Environment	Conc. (mg/L)	Temp (°C)	ThOD	28 days	Other	Rates coefficients	Half-life (d)	Project	Laboratory	Reference
Acetic acid 64-19-7	Study with 14C-acetic acid	Primary (depletion)	Soil	34	20	Not relevant			0,346500	2,0		Review	ECHA dossier
Oxalic acid 144-62-7	BOD	Ultimate	Activated sludge	10	20	No infor		d5: 89%	0,441455	1,6		Review	ECHA dossier
Bicine 150-25-4	OECD301F-manometric	Ultimate	Activated sludge	48	20		94	d14: 77%	0,104977	6,6		Review	ECHA dossier
1-hydroxyetane-1,1-diphosphonic acid (HEPD) 2809-21-4	OECD301D-BOD	Ultimate	Activated sludge	120	20		15		0,005804	119,4		Review	ECHA dossier
N-(2-hydroxyethyl)glycine (HeGly) 5835-28-9	No data												
Ammonia 7664-41-7	Not relevant												
Ammonium chloride 12125-02-9	Not relevant												
Formaldehyde 50-00-0	OECD301A-TOC OECD301C-BOD	Ultimate Ultimate	Activated sludge Activated sludge	20 20	20 20	1,07 1,07	99	d14: 91	0,164470 0,171996	4,2 4,0		Review Review	ECHA dossier ECHA dossier
Acetaldehyde 75-07-0	OECD301C-BOD	Ultimate	Domestic sewage	100	20	1,82		d14: 80	0,114960	6,0		Review	ECHA dossier
Ethylene glycol 107-21-1	OECD301C-BOD OECD301A-DOC	Ultimate Ultimate	Sewage/soil No information	No information No information	20 20			d14: 83% d10: >90%	0,126568 0,230259	5,5 3,0		Review Review	ECHA dossier ECHA dossier
Acetone 67-64-1	OECD301B-CO2 APHA 219-BOD BOD-test	Ultimate Ultimate Ultimate	No information No information saltwater with adapted bact.	No information No information No information	20 20 20		91	d5: 84% d20: 76%	0,085998 0,366516 0,071356	8,1 1,9 9,7		Review Review Review	ECHA dossier ECHA dossier ECHA dossier
Acetonitrile 75-05-8	No information BOD-test				20			d14: 30%	0,025477	27,2		Review Risk report on acetonitrile	ECHA dossier EC, 2010
Methylamine 74-89-5	OECD301C-TOC OECD301F-manometric	Ultimate Ultimate	Activated sludge Activated sludge	100 400	20 20	1,42 3,09	96 55		0,114960 0,028518	6,0 24,3		Review Review	ECHA dossier ECHA dossier
Dimethylamine 124-40-3	OECD301C-TOC OECD306	Ultimate Ultimate	Activated sludge Seawater	100 2	20 20	1,42 1,42	96 77		0,114960 0,052488	6,0 13,2	REACT	Review SINTEF	ECHA dossier Eide-Haugmo, 2012
Ethylamine 75-04-7	OECD301C-BOD	Ultimate	Sludge, soil and water	No information	20		90		0,082235	8,4		Review	ECHA dossier

Name and CAS	Method	Degradation	Environment	Conc. (mg/L)	Temp (°C)	ThOD	28 days	Other	Rates coefficients	Half-life (d)	Project	Laboratory	Reference
Diethylamine 109-89-7	OECD301C-BOD	Ultimate	Activated sludge	No information	20		69		0,041828	16,6		Review	ECHA dossier
	OECD301F-BOD	Ultimate	Activated sludge	No information	20		67		0,039595	17,5		Review	ECHA dossier
Ethyl-methylamine 624-78-2	OECD301D-BOD	Ultimate	No information	No information	20		67		0,039595	17,5		Review	ECHA dossier
Propylamine 107-10-8	OECD310-CO2	Ultimate	Activated sludge	No information	20		78		0,054076	12,8		Review	ECHA dossier
2-methyl-2-(methylamino)propane-1-ol 27646-80-6	No information											Review	ECHA dossier
Nitromethane 75-52-5	OECD301D-BOD	Ultimate	No information	No information	20		<10		0,003763	184,2		Review	ECHA dossier
Nitroethane 79-24-3	OECD301D-BOD	Ultimate	No information	No information	20		<1		0,000359	1930,7		Review	ECHA dossier
	Not standard-CO2	Ultimate	No information	0,05	20?			d5: 24%	0,054887	12,6		Review	ECHA dossier
N-(2-hydroxyethyl)-ethylenediamine (HEED) 111-41-1	No information OECD301C	Ultimate	No information	No information	20		1		0,000359	1930,7		Review Sigma_Aldrich	ECHA dossier HSE sheet
Formamide 75-12-7	OECD301A-DOC	Ultimate	No information	No information	20		>60%		0,032725	21,2		Review	ECHA dossier
Acetamide 60-35-5	OECD301D-BOD		No information	No information	20			d11: 69%	0,106471	6,5		Review	ECHA dossier
N-(2-hydroxyethyl)-formamide (HEF) 693-06-1	No information											Review	ECHA dossier
N-(2-hydroxyethyl)acetamide (HEA) 142-26-7	OECD301D-BOD	Ultimate	Activated sludge	2	20		48		0,023355	29,7		Review	ECHA Dossier
Hydroxyethyl acetamide (HEHEAA) 144236-39-5	No data												
N,N'-bis(2-hydroxyethyl) oxamide (BHEOX) 1871-89-2	No data												
Piperazine 110-85-0	OECD301F-manometric	Ultimate	Activated sludge	28	20		39		0,017653	39,3		Review	ECHA Dossier
	OECD301D-BOD	Ultimate	Freshwater	2	20		<1		0,000359	1930,7	CESAR	SINTEF	Brakstad et al., 2010
	OECD306-BOD	Ultimate	Seawater	2	20		3		0,001088	637,0	REACT	SINTEF	Eide-Haugmo, 2012
	LC-MS	Primary	Freshwater		20		97		0,125234	5,5	SOLVit	SINTEF	Brakstad et al., 2012
	LC-MS	Primary	Freshwater		10		54,5		0,028123	24,6	SOLVit	SINTEF	Brakstad et al., 2012
LC-MS	Primary	Freshwater		5		11,9		0,004525	153,2	SOLVit	SINTEF	Brakstad et al., 2012	

Name and CAS	Method	Degradation	Environment	Conc. (mg/L)	Temp (°C)	ThOD	28 days	Other	Rates coefficients	Half-life (d)	Project	Laboratory	Reference
4-hydroxyethyl)piperazin-2-one 23936-04-1	No data												
Morpholine 110-91-8	OECD301E-DOC OECD306-BOD	Ultimate Ultimate	Activated sludge Seawater	No information 2	20 20		92 22		0,090205 0,008874	7,7 78,1	REACT	Review SINTEF	ECHA Dossier Eide-Haugmo, 2012
4-acetomorpholine 1696-20-4	OECD302B	Inherent	Activated sludge	No information	20		>60%		0,032725	21,2		Review	ECHA dossier
Imidazole 288-32-4	OECD301A-DOC OECD301C-BOD	Ultimate Ultimate	Activated sludge Activated sludge	No information No information	20 20			d18: 90% 90	0,127921 0,082235	5,4 8,4		Review Review	ECHA dossier ECHA dossier
N-(2-hydroxyethyl)imidazole (HEI) 1615-14-1	No information											Review	ECHA dossier
1-(2-hydroxyethyl)-2-imidazolidone (HEIA) 3699-54-5	ISO7827-DOC OECD302C	Ultimate Inherent	No information No information	No information No information	20 20		1		0,000359 0,065449	1930,7 10,6		Review Review	ECHA dossier ECHA dossier
Pyrrrole 109-97-7	OECD301E-DOC OECD306-BOD	Ultimate Ultimate	Activated sludge Seawater	No information 2	20 20			d9: 95% ND	0,332859 0,067754	2,1 10,2	REACT	Review SINTEF	ECHA Dossier Eide-Haugmo, 2012
1,1'-(1,3-phenylene)bis-1H-pyrrole-2,5-dione 119462-56-5	No information	Ultimate	No information	No information	20		1		0,000359	1930,7		Review	ECHA dossier
Pyrazine 290-37-9	No information											Review	ECHA dossier
Methylpyrazine 109-08-0	No information											Review	ECHA dossier
Dimethylpyrazine 123-32-0	No information OECD306	Ultimate	Seawater	No information	20		22		0,008874	78,1		Review UoStavanger	ECHA dossier
Oxazolidinone 497-25-6	No information											Review	ECHA dossier
4,4-dimethyloxazolidinone 26654-39-7	No information											Review	ECHA dossier
N-nitrosodiethanolamine (NDELA) 1116-54-7	OECD301D-BOD Mod OECD309-LCMS Mod OECD309-LCMS Mod OECD309-LCMS Mod OECD308-LCMS	Ultimate Primary Primary Primary Primary	Lake and river water Lake and river water Lake and river water Lake and river water water/sediment (anaerobic)	2 0,001 0,001 0,001 0,2	20 20 10 5 20	1,55 Not relevant Not relevant Not relevant Not relevant	17	d56: 68% d56: 62 d56: 50 d21: 55%	0,006655 0,020347 0,017278 0,012378 0,038024	104,1 34,1 40,1 56,0 18,2	TCM, 2011 TCM, 2011 TCM, 2011 TCM, 2011 Solvate, 2014	SINTEF SINTEF SINTEF SINTEF SINTEF	Brakstad et al., 2011a Brakstad et al., 2011b Brakstad et al., 2011b Brakstad et al., 2011b Booth et al., 2014
Name and CAS	Method	Degradation	Environment	Conc. (mg/L)	Temp (°C)	ThOD	28 days	Other	Rates coefficients	Half-life (d)	Project	Laboratory	Reference

Nitrosopiperidine (NPIP) 140-79-4	OECD301D-BOD	Ultimate	Lake and river water	2	20	2,38	1		0,000359	1930,7	TCM, 2011	SINTEF	Brakstad et al., 2011a
Name and CAS	Method	Degradation	Environment	Conc. (mg/L)	Temp (°C)	ThOD	28 days	Other	Rates coefficients	Half-life (d)	Project	Laboratory	Reference
Nitrosodiethylamine (NDEA) 55-18-5	OECD301D-BOD	Ultimate	Lake and river water	2	20	2,35	1		0,000359	1930,7	TCM, 2011	SINTEF	Brakstad et al., 2011a
Name and CAS	Method	Degradation	Environment	Conc. (mg/L)	Temp (°C)	ThOD	28 days	Other	Rates coefficients	Half-life (d)	Project	Laboratory	Reference
Nitrosodimethylamine (NDMA) 62-75-9	OECD301D-BOD	Ultimate	Lake and river water	2	20	1,94	1		0,000359	1930,7	TCM, 2011	SINTEF	Brakstad et al., 2011a
	Mod OECD309-LCMS	Primary	Lake and river water	0,005	20	Not relevant		d56: 5%	0,000916	756,6	TCM, 2011	SINTEF	Brakstad et al., 2011b
	Mod OECD308-LCMS	Primary	water/sediment (anaerobic)	0,1	20	Not relevant		d49: 1%	0,000205	3378,7	Solvfate, 2014	SINTEF	Booth et al., 2014
Name and CAS	Method	Degradation	Environment	Conc. (mg/L)	Temp (°C)	ThOD	28 days	Other	Rates coefficients	Half-life (d)	Project	Laboratory	Reference
Nitroso-N-methylethylamine (NMEA) 10595-95-6	OECD301D-BOD	Ultimate	Lake and river water	2	20	2,18	1		0,000359	1930,7	TCM, 2011	SINTEF	Brakstad et al., 2011a
Name and CAS	Method	Degradation	Environment	Conc. (mg/L)	Temp (°C)	ThOD	28 days	Other	Rates coefficients	Half-life (d)	Project	Laboratory	Reference
Nitrosomorpholine (NMOR) 59-89-2	OECD301D-BOD	Ultimate	Lake and river water	2	20	1,79	1		0,000359	1930,7	TCM, 2011	SINTEF	Brakstad et al., 2011a
Name and CAS	Method	Degradation	Environment	Conc. (mg/L)	Temp (°C)	ThOD	28 days	Other	Rates coefficients	Half-life (d)	Project	Laboratory	Reference
Nitroso-N-dipropylamine (NDPA) 621-64-7	OECD301D-BOD	Ultimate	Lake and river water	2	20	2,58	1		0,000359	1930,7	TCM, 2011	SINTEF	Brakstad et al., 2011a
Name and CAS	Method	Degradation	Environment	Conc. (mg/L)	Temp (°C)	ThOD	28 days	Other	Rates coefficients	Half-life (d)	Project	Laboratory	Reference
Nitrosopyrrolidone (NPYR) 930-55-2	OECD301D-BOD	Ultimate	Lake and river water	2	20	2,24	1		0,000359	1930,7	TCM, 2011	SINTEF	Brakstad et al., 2011a
Name and CAS	Method	Degradation	Environment	Conc. (mg/L)	Temp (°C)	ThOD	28 days	Other	Rates coefficients	Half-life (d)	Project	Laboratory	Reference
Nitrosopiperazine (NPZ) 5632-47-3	OECD301D-BOD	Ultimate	Lake and river water	2	20	2,22	1		0,000359	1930,7	TCM, 2011	SINTEF	Brakstad et al., 2011a
	Mod OECD309-LCMS	Primary	Lake and river water	0,01	20	Not relevant		d56: 1%			TCM, 2011	SINTEF	Brakstad et al., 2011b
Name and CAS	Method	Degradation	Environment	Conc. (mg/L)	Temp (°C)	ThOD	28 days	Other	Rates coefficients	Half-life (d)	Project	Laboratory	Reference
Dinitrosoperazine (DNPZ) 140-79-4	OECD301D-BOD	Ultimate	Lake and river water	2	20	1,78	1		0,000359	1930,7	TCM, 2011	SINTEF	Brakstad et al., 2011a
Name and CAS	Method	Degradation	Environment	Conc. (mg/L)	Temp (°C)	ThOD	28 days	Other	Rates coefficients	Half-life (d)	Project	Laboratory	Reference
Nitroso(2-hydroxy)glycine (NO-HeGly) 80556-89-4	No data												
Name and CAS	Method	Degradation	Environment	Conc. (mg/L)	Temp (°C)	ThOD	28 days	Other	Rates coefficients	Half-life (d)	Project	Laboratory	Reference
Dimethylnitramine (DMNA) 4164-28-7	Mod OECD309-LCMS	Primary	Lake and river water	0,002	20	Not relevant			0,01829	37,9	TCM, 2014	SINTEF	Brakstad et al., 2014
	OECD301D-BOD	Ultimate	Lake and river water	2	20	1,42	3,4		0,001235	560,9	TQPAmine5, 2011	SINTEF	Dye et al., 2011
	Mod OECD308-LCMS	Primary	water/sediment (anaerobic)	0,1	20	Not relevant		d49: 18%	0,004050	171,1	Solvfate, 2014	SINTEF	Booth et al., 2014
Name and CAS	Method	Degradation	Environment	Conc. (mg/L)	Temp (°C)	ThOD	28 days	Other	Rates coefficients	Half-life (d)	Project	Laboratory	Reference
Ethanolnitramine (MEA-NO2) 74386-82-6	Mod OECD309-LCMS	Primary	Lake and river water	0,02	20	Not relevant			0,08319	28,7	TCM, 2014	SINTEF	Brakstad et al., 2014
	OECD301D-BOD	Ultimate	Lake and river water	2	20	1,06	33		0,014303	48,5	TQPAmine5, 2011	SINTEF	Dye et al., 2011
	Mod OECD308-LCMS	Primary	water/sediment (anaerobic)	0,1	20	Not relevant		d21: 85%	0,090339	7,7	Solvfate, 2014	SINTEF	Booth et al., 2014
Name and CAS	Method	Degradation	Environment	Conc. (mg/L)	Temp (°C)	ThOD	28 days	Other	Rates coefficients	Half-life (d)	Project	Laboratory	Reference
Methylnitramine (MNA) 598-57-2	Mod OECD309-LCMS	Primary	Lake and river water	0,05	20	Not relevant	1		0,000359	1930,7	TCM, 2014	SINTEF	Brakstad et al., 2014
	OECD301D-BOD	Ultimate	Lake and river water	2	20	1,05	34		0,014840	46,7			
Name and CAS	Method	Degradation	Environment	Conc. (mg/L)	Temp (°C)	ThOD	28 days	Other	Rates coefficients	Half-life (d)	Project	Laboratory	Reference
1-nitropiperazine (PZ-NO2) 42499-41-2	Mod OECD309-LCMS	Primary	Lake and river water	0,02	20	Not relevant	1		0,000359	1930,7	TCM, 2014	SINTEF	Brakstad et al., 2014
	OECD301D-BOD	Ultimate	Lake and river water	2	20	1,5	3		0,001088	637,0	TQPAmine5, 2011	SINTEF	Dye et al., 2011
Name and CAS	Method	Degradation	Environment	Conc. (mg/L)	Temp (°C)	ThOD	28 days	Other	Rates coefficients	Half-life (d)	Project	Laboratory	Reference
1-methyl-2-(nitroamino)-1-propanol (AMP-NO2) 1239666-60-4	Mod OECD309-LCMS	Primary	Lake and river water	0,02	20	Not relevant			0,05256	38,7	TCM, 2014	SINTEF	Brakstad et al., 2014
	OECD301D-BOD	Ultimate	Lake and river water	2	20	1,55	20		0,007969	87,0	TQPAmine5, 2011	SINTEF	Dye et al., 2011

Name and CAS	Method	Degradation	Environment	Conc. (mg/L)	Temp (°C)	ThOD	28 days	Other	Rates coefficients	Half-life (d)	Project	Laboratory	Reference
Diethylnitramine (DENA) 7119-92-8	Mod OECD309-LCMS	Primary	Lake and river water	0,05	20	Not relevant	1		0,000359	1930,7	TCM, 2014	SINTEF	Brakstad et al., 2014