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ACRYLONITRILE

CAS No: 107-13-1

EINECS No: 203-466-5

Summary Risk Assessment Report

2004 **Special Publication I.03.157**

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SUMMARY RISK ASSESSMENT REPORT

Final report 2004

Ireland

The risk assessment of acrylonitrile has been prepared by Ireland on behalf of the European Union. The scientific work contained in the report has been prepared by the Hazardous Substances Assessment Unit of the Health and Safety Authority.

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PREFACE

This report provides a summary, with conclusions, of the risk assessment report of the substance acrylonitrile that has been prepared by Ireland in the context of Council Regulation (EEC) No. 793/93 on the evaluation and control of existing substances.

For detailed information on the risk assessment principles and procedures followed, the underlying data and the literature references the reader is referred to the comprehensive Final Risk Assessment Report (Final RAR) that can be obtained from the European Chemicals Bureau[1]. The Final RAR should be used for citation purposes rather than this present Summary Report.

[1] European Chemicals Bureau – Existing Chemicals – http://ecb.jrc.it

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1 GENERAL SUBSTANCE INFORMATION

1.1 IDENTIFICATION OF THE SUBSTANCE

CAS Number: 107-13-1
EINECS Number: 203-466-5
IUPAC Name: 2-propenenitrile
Synonyms: Vinyl cyanide, cyanoethylene, acrylonitrile
Molecular weight: 53.06
Molecular formula: C_3H_3N
Structural formula: $CH_2 = CH - CN$

1.2 PHYSICO-CHEMICAL PROPERTIES

Table 1.1 Summary of physico-chemical properties

Property	Value
Physical state	Colourless liquid
Solidifying Point	- 83.55°C * ± 0.5°C
Boiling point	77.3°C *
Relative Density	0.8060 at 20°C
Vapour Pressure	115 hPa at 20°C 133.3 hPa at 22.8°C *
Surface tension	27.3 mN/m at 24°C
Water solubility	73.5 g/l at 20°C *
Partition coefficient (log Pow)	0.25 *
Flash point	0°C (open cup method) -5°C (open cup method)
Autoflammability	481°C

* value used in the assessment of environmental exposure in this report

1.3 CLASSIFICATION

Classification and labelling according to the 26th ATP of Directive 67/548/EEC[2]:

Classification

F; R11	Highly flammable
Carc. Cat.2; R45	May cause cancer
T; R23/24/25	Also toxic by inhalation, in contact with skin and if swallowed
Xi; R37/38-41	Irritating to respiratory system and skin. Risks of serious damages to eyes
R43	May cause sensitisation by skin contact
N; R51-53	Dangerous for the environment, toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment

Notes: D, E

Labelling

F; T; N
R 45-11-23/24/25-37/38-41-43-51/53
S 9-16-53-45-61

Specific concentration limits

C ≥ 20%	T; R45-23/24/25-37/38-41-43
10%≤C<20%	T; R45-23/24/25-41-43
5%≤C<10%	T; R45-23/24/25-36-43
1%≤C< 5%	T; R45-23/24/25-43
0.2%≤C< 1%	T; R45-20/21/22
0.1%≤C<0.2%	T; R45

[2] The classification of the substance is established by Commission Directive 2000/32/EC of 19 May 2000 adapting to technical progress for the 26th time Council Directive 67/548 on the approximation of the laws, regulations and administrative provisions relating to the classification, packaging and labelling of dangerous substances.

2 GENERAL INFORMATION ON EXPOSURE

Production of acrylonitrile in the European Union over the period 1994-1996 was in excess of 1,250,000 tonnes per annum (source PCI World Acrylonitrile Report, 1996). Acrylonitrile is produced from ammonia and propylene via catalytic ammoxidation in a closed system. It is used almost exclusively as a monomer in the production of polymeric materials, with some use as a precursor in the production of acrylamide and adiponitrile. Approximately 52% of the total EU production of acrylonitrile is used for the production of acrylic and modacrylic textile fibres, used in clothing and domestic furnishings. Production of acrylonitrile-butadiene-styrene (ABS) and styrene-acrylonitrile (SAN) plastics, used in automotive parts, household appliances, pipe fittings, containers for food, etc. accounts for 15% of use, while a further 15% is used in the production of acrylamide and adiponitrile and 18% for other uses, including production of nitrile rubber and other polymeric materials.

At the time that data were collected for the purposes of this risk assessment, in 1994–1996, acrylonitrile was produced by 7 manufacturers at 8 sites in the European Union, located in Germany, Italy, Netherlands, Spain and the United Kingdom. Although production takes place in closed systems in a largely continuous process, start-up, shut-down, product recovery and purification steps result in some release of acrylonitrile to air or water. Production wastes are however either incinerated, or treated by for example gas scrubbing of emissions followed by release of scrubber washes to wastewater, thus significantly reducing the environmental emissions. Tank breathing during storage is a further source of releases to atmosphere.

Data provided by the PCI World Acrylonitrile and Derivatives Supply/Demand Report (1996) indicated that at that time there were 11 major facilities producing acrylic fibres throughout Western Europe, two of which ceased production in 1996/97, 13 facilities producing ABS/SAN plastics, 10 facilities producing nitrile:butadiene copolymers, 3 facilities producing acrylamide and 1 producing adiponitrile. Limited (drum) quantities of acrylonitrile are used by a number of small companies in Europe. The estimate for drummed product for the whole European Union market is less than 1,000 tonnes, on a total production tonnage of 1,250,000 tonnes, or less than 0.1%. As for production, polymerisation of acrylonitrile is carried out in largely closed systems, using broadly similar polymerisation processes, however start-up, shut-down, product recovery and washing steps result in some release of acrylonitrile to air or water. Following polymerisation, unreacted monomer is recovered and recycled to the reactor.

Subsequent processing steps involving acrylonitrile in polymerised form, e.g. drying, dyeing of fibres or use in textile manufacture, shaping of acrylonitrile plastics and rubbers, are assumed to result in relatively minor releases of free acrylonitrile compared with the initial polymerisation and processing steps, given the low content of residual monomer.

Releases of acrylonitrile within production and processing facilities can result in exposure of workers, while releases to atmosphere and water can lead to exposure of the environment and consequently to man exposed via the environment. Vehicle exhausts have been reported to represent a significant source of diffuse emissions of acrylonitrile to air, while cigarette smoke represents a minor source. Consumers may potentially be exposed via use or wearing of materials which may contain a small percentage of unreacted monomer, or via the food which is packaged in containers made from acrylonitrile derived plastics. In practice, data gathered for the risk assessment report indicates that consumer exposure is extremely low.

3 ENVIRONMENT

3.1 ENVIRONMENTAL EXPOSURE

Exposure of the aquatic compartment to acrylonitrile may occur as a result of release to water during production of monomer, polymerisation of monomer to give acrylonitrile polymers, further processing of polymer to give polymeric products, use and, ultimately, disposal of the polymeric products. Exposure on a local scale is to a limited (multiple) number of point sources involved in the large-scale production of acrylonitrile and/or further processing of acrylonitrile polymers. Exposure to acrylonitrile as a result of disposal of polymeric products to landfill for example, with subsequent release to the aquatic environment, is considered to be insignificant compared with manufacturing point sources. Emissions from vehicle exhausts and other diffuse sources, as mentioned in Section 2 are largely to atmosphere rather than the aquatic compartment. Tank breathing during storage is a further source of releases to atmosphere. Modelling of environmental distribution using measured values for vapour pressure, water solubility, log P_{ow} and other physicochemical properties and a value of 9.62 $Pa/m^3/mol$ for Henry's law constant indicates that the predicted major environmental compartment for acrylonitrile is air, with a smaller proportion entering the aqueous compartment and negligible quantities being predicted for other compartments.

The total releases from all currently operational production and processing plants provide a figure of approximately 400 tonnes per annum acrylonitrile released to water, on a production volume of approximately 1,250,000 tonnes per annum. The point source releases to air for continental releases at a European level have been estimated to total 900 tonnes per annum. Indirect emissions due to e.g. vehicle exhausts may contribute as much as 2,400 tonnes per annum of acrylonitrile, although this is considered to represent a worst-case analysis.

In relation to exposure assessment for the aquatic environment, the currently operational production and further processing companies can be divided into three groups:

1. Facilities with dedicated industrial wastewater treatment plants,
2. Two facilities discharging into a municipal wastewater treatment plant following preliminary physicochemical treatment to recover acrylonitrile from waste,
3. Facilities discharging directly into the aquatic environment (river/marine/estuarine) without biotreatment.

In the case of group (1), which represents a large proportion of total sites (33 out of a total of 43), the results of laboratory-scale simulation studies and other information indicate that acrylonitrile may be regarded as readily biodegradable in this situation. In the case of groups (2) and (3) it is regarded as inherently biodegradable. Following release to the environment, acrylonitrile is thus degraded in water, and also in the atmosphere and in soil. Photolytic degradation in water has also been reported. In relation to atmospheric degradation the published rate constant for the reaction of acrylonitrile with $OH^{\cdot}$ of $3.2 \cdot 10^{-12}$cm/mol/s has been used in EUSES, representing an estimated half-life of 5 days in the troposphere. Experimental data for biodegradation provide values for the half-life ranging from 2 days in a fully acclimated system to 15 days in a ready biodegradability test in seawater and 30 days in a standard ready biodegradability test. Transfer of acrylonitrile from the aqueous to the atmospheric compartment can potentially arise as a consequence of volatilisation and air stripping from WWTP, given the relatively high vapour pressure of acrylonitrile. However this is counterbalanced by its high water solubility.

Bioaccumulation of acrylonitrile is not anticipated, given experimentally derived values of 0-0.3 for the log Kow, and a bioconcentration factor (BCF) of 1.0 has been calculated from the known water solubility of acrylonitrile. EUSES calculates a BCF for fish and aquatic biota of 1.41 L/kg.

PEC calculations

PECs were calculated using the approach outlined in the EU Technical Guidance for Risk Assessment of New and Existing Chemicals, assuming, where appropriate, initial on-site STP treatment followed by release to a municipal STP or surface water. Local PEC values calculated for the aquatic compartment and for air for individual production and processing facilities are reproduced in the Appendix.

The following results were obtained for regional and continental PECs for water and air:

$PECregional_{water}$	2.81 µg/l	$PECcontinental_{water}$	0.41 µg/l
$PECregional_{air}$	$7.08 \cdot 10^{-5}$ mg/m^3	$PECcontinental_{air}$	$2.49 \cdot 10^{-5}$ mg/m^3

Monitoring data indicate that concentrations of acrylonitrile in surface waters are generally below the limit of detection of 1-2 µg/l. In relation to measured levels of acrylonitrile in air, a study of acrylonitrile in urban German air over the period 1977–1984 indicated levels of between 0.01-10.4 µg/m^3, while clean (rural) air contained less than 0.002 µg/m^3. Acrylonitrile was not detected over a 6-month monitoring period of urbanised and industrialised air in the Gulf Coast of Texas (limit of detection 0.122 µg/m^3).

In relation to the terrestrial compartment, the $PEClocal_{soil}$ was calculated assuming sludge from a WWTP containing acrylonitrile was applied to soil once a year for 10 years, to which was added the contribution loads from wet and dry deposition. The result for $PEClocal_{soil}$ for processing sites was 3.86 µg/kg wet weight (wwt) averaged over 30 days or 180 days. The value for production was 0.17 mg/kg wet weight averaged over 30 days or 0.046 mg/kg wet weight averaged 180 days, while PEC_{local} in soil pore water (agricultural soil) was 0.3 mg/kg wwt. It should be noted, however, that this is a worst-case exposure scenario, and appears unrealistic, given the information from industry that little industrial sludge from acrylonitrile production and processing facilities is spread on land in Europe. The majority of companies providing information on this aspect indicated that contaminated sludge is incinerated together with other wastes. The conclusion however cannot be extrapolated to sites not covered by this risk assessment. Given the very low levels of acrylonitrile anticipated to be present in the terrestrial environment, no significant levels are expected in plants or other terrestrial species, potential routes of exposure being deposition from air or contaminated effluents or surface waters.

EUSES provides values for exposed biota, as follows:

Regional concentration in wet fish, mg/kg:	$3.96 \cdot 10^{-3}$
Regional concentration in plant root tissue, mg/kg:	$1.3 \cdot 10^{-4}$
Regional concentration in plant leaves, mg/kg:	$1.66 \cdot 10^{-5}$
Regional concentration in grass, mg/kg:	$1.66 \cdot 10^{-5}$
Regional concentration in meat (wet weight), mg/kg:	$1.30 \cdot 10^{-7}$
Regional concentration in milk (wet weight), mg/kg:	$1.30 \cdot 10^{-6}$

EUSES also provides values for daily human intake from the environment, as follows:

Daily intake through drinking water (mg/kg/day):	$8.01 \cdot 10^{-5}$
Daily intake through consumption of fish (mg/kg/day):	$6.51 \cdot 10^{-6}$
Daily intake through consumption of leaf crops (mg/kg/day):	$2.84 \cdot 10^{-7}$
Daily intake through consumption of root crops (mg/kg/day):	$7.12 \cdot 10^{-7}$
Daily intake through consumption of meat (mg/kg/day):	$5.61 \cdot 10^{-10}$
Daily intake through consumption of milk (mg/kg/day):	$1.04 \cdot 10^{-8}$
Daily intake through intake of air (mg/kg/day):	$1.52 \cdot 10^{-5}$
Regional total daily intake for humans (mg/kg/day)	$1.03 \cdot 10^{-4}$

It is concluded from these results that the potential for secondary poisoning is very small.

3.2 EFFECTS ASSESSMENT

Acrylonitrile is toxic to aquatic organisms. Valid short-term L(E)C_{50}s for acrylonitrile have been reported for fish, Daphnia, algae and microorganisms. The most reliable result in fish is considered to be that in the saltwater species *Cyprinodon variegatus* in which a 96-hour LC_{50} of 8.6 mg/l was reported. The absolute validity of the lower figure of 5.2 mg/l for *Ctenophayngodon idellus* cannot be ascertained. The lowest 48-hour EC_{50} for Daphnia was 7.6 mg/l (nominal concentration, *Daphnia magna*). Two valid results are available for the 72-hour EC_{50} (biomass) in algae, 2.5 mg/l in *Scenedesmus subspicatus* and 1.63 mg/l (measured concentration at t_0) in the saltwater diatom *Skeletonema costatum*.

Long-term toxicity data are available in fish, Daphnia and algae. The fish early life stage toxicity test in *Pimephales promelas*, using flow-through conditions, provided a LOEC/NOEC of 0.34 mg/l, while a 30-day flow through test in mature fish of the same species provided a long-term LC_{50} of 2.6 mg/l. If the value of 0.34 mg/l is taken as a LOEC, a NOEC may be derived by application of a safety factor of 2, giving a NOEC of 0.17 mg/l. The 14/21-day life cycle study in *Daphnia magna* provided a NOEC of 0.5 mg/l (nominal), while NOECs for effects on biomass in algae are reported as 0.8 mg/l (*Scenedesmus subspicatus*) and 0.41 mg/l (*Skeletonema costatum*). For risk characterisation purposes, a PNEC has been derived using an assessment factor of 10. Applying this factor to the NOEC derived from the fish early life stage toxicity test in *Pimephales promelas* gives a PNEC of 17 μg/l.

The results of microbial toxicity tests and biodegradation studies on acrylonitrile indicate a potential effect on microorganisms in wastewater treatment plants, at least on start-up. The reported EC_{50}s range from 1 - > 1,800 mg/l. Results with acclimated microbial populations and in simulation tests have indicated no inhibitory effect of acrylonitrile at levels as high as 200 mg/l, and a conservative estimate of 50 mg/l for a NOEC in such populations has been assumed. Application of a factor of 10 to this NOEC derives a PNEC of 5 mg/l for microorganisms in acclimated wastewater treatment plants handling acrylonitrile on a continuous basis. A factor of 10 is considered justified given the relatively large body of data on microbial toxicity of acrylonitrile.

$PEC_{sediment}$ and $PNEC_{sediment}$ can be derived from the results for water. A PNEC for sediment of 0.0126 mg/kg (based on PNEC (aquatic) of 17 μg/l) was derived using the above approach. A PNEC for soil of 0.00268 mg/kg was derived, based on PNEC (aquatic) of 17 μg/l. The reported NOEC for soil microorganisms is comparatively high, at approximately 100 mg/kg, providing a PNEC of 100 μg/kg (assessment factor 1,000). Data available for derivation of a

PNEC for non-soil-dwelling terrestrial organisms are limited and of unknown quality. Using the LC_{50} data generated in a number of insect species and assuming a conservative figure of 0.5 mg/l for the LC_{50} gives a PNEC of 0.5 μg/l air

3.3 RISK CHARACTERISATION

Acrylonitrile is toxic to aquatic organisms and is not readily biodegradable. Release into the aquatic environment could therefore possibly present some risk to aquatic species in the vicinity of plants producing or further processing acrylonitrile. Information from simulation tests and on the performance of wastewater biotreatment plants in a number of companies indicates that greater than 90% biodegradation is achieved in acclimated WWTPs. Of the 43 companies producing or processing acrylonitrile in the European Union, 33 have dedicated industrial WWTPs and a further 2 discharge to municipal WWTP. The PEC:PNEC ratio for the aquatic compartment (water and sediment) for all but 1 of these 43 companies is below 1.0, indicating that the risk is adequately managed by the control measures in place. In the case of one site, located on a large marine estuary, application of a specific dilution factor of 701 derived from modelling of the dilution due to seawater results in a PEC:PNEC ratio of 3.1 for water and 3.46 for sediment. It is concluded that there are concerns for possible effects on the local aquatic environmental sphere as a consequence of exposure arising from production of acrylic fibres at this site only.[3] It should be noted, however, that this conclusion applies only at a particular point in time to 42 out of the total of 43 European sites existing at the time and which provided aquatic release data relating to the period 1994-1996, and cannot be extrapolated generally for the aquatic environment. The specific risk reduction measures (eg wastewater treatment) or particular characteristics of the assessed sites (e.g. high dilution factors due to effluent emissions into very large rivers or estuaries) cannot be extrapolated to sites not covered by this risk assessment, for example new sites starting up after the data for this assessment were gathered, or sites located outside the European Union.

In relation to risk assessment for microorganisms in wastewater treatment plants, a PNEC of 5 mg/l is estimated for sites with acclimatised WWTPs, while for non-acclimated WWTPS a PNEC of 100 μg/l was derived. For sites with WWTP which produced measured data for effluent, concentrations ranged from 0 to 5.8 mg/l. Appendices A and B show that the PEC:PNEC ratios for sites having WWTP are all below 1.0. It can be concluded that there is little or no risk for microorganisms in industrial WWTP, although some risk may exist in non-acclimated WWTP. In practice the companies providing data for this report have indicated that, in the main, their WWTPs operate continually and are fully acclimatised to acrylonitrile waste.

[3] Since the publication of the risk assessment, the site in question has participated with the relevant national authority in working on a risk reduction programme. The aim of the programme was to first quantify the risk by measuring actual acrylonitrile in the receiving waters. A modelling and sampling exercise took place in 2000 using a team of independent consultants approved by the Authorities. The position of the effluent plume was determined using a number of techniques including dye tracing, drogue tracking and analysis of species known to be present in the effluent. Effluent samples were taken in the effluent plume on two separate occasions at distances between 100 and 5,000 m from the effluent discharge pipe. The level of acrylonitrile present in all samples was below the analytical detection limit of 1.3 μg/l and therefore well below the PNEC of 17 μg/l. The most plausible explanation for the results to date is that acrylonitrile in the effluent is being degraded rapidly by bacteria that have become acclimatised to using acrylonitrile as a food source. Sediment samples taken during the survey proved that the benthic fauna composition was as expected and healthy. At a meeting with the authorities, it was agreed that a future work programme might include another survey to determine if changes to the make up of the production units on the site have made any difference to the results.

Although the atmospheric compartment is the major compartment of distribution of acrylonitrile, there is rapid photodegradation ($t_{1/2}$ approximately 5 days). Local emissions from production and processing facilities can be predicted to give rise to the highest atmospheric concentrations, and the calculated $PEClocal_{air}$ for sites providing specific emission data lies between 0 and 0.240 mg/m^3 or 1-240 µg/l. Results of monitoring at the perimeter of acrylonitrile plants shows that levels are generally below 1 µg/m^3. No effect information is available, other than the effects of acrylonitrile on a number of insect species known to infest food, which showed an LC_{50} of 0.5 mg/l, and therefore a PNEC of 0.5 µg/l. However the quality of these studies is questionable, and also taking into account the measured levels in the vicinity of plants it is concluded that there is little risk associated with exposure of ecosystems to atmospheric environmental levels of acrylonitrile. The PEC:PNEC ratios for air are all below 1.0.

In relation to the terrestrial compartment, the estimate of $PECregional_{soil}$ reflects primarily point source emissions from production or further processing, and diffuse emissions from car exhausts etc. have not been taken into account in the EUSES input. However, even with a significant contribution to $PECregional_{soil}$ from such sources, the PEC:PNEC ratio will still be well below 1, again indicating little concern for this compartment.

4 HUMAN HEALTH

4.1 HUMAN HEALTH (TOXICITY)

4.1.1 Exposure assessment

The human population may be exposed to acrylonitrile at the workplace, and to a minimal/negligible extent indirectly via the environment. Exposure of consumers is also possible, via use or wearing of materials which may contain a small percentage of unreacted acrylonitrile monomer, or via food which is packaged in containers made from acrylonitrile-derived plastics.

Occupational exposure

Acrylonitrile is released during industrial production and processing to air and wastewater. The main human exposure is via air (inhalation) regarding occupationally exposed workers. As acrylonitrile is produced and almost totally processed in a closed system, the main concern relating to exposure relates to the accident scenario or due to breaches in the closed system. The 8-hour time-weighted average Occupational Exposure Limit in the majority of countries having such a limit is between 2 and 3 ppm. Only 3 countries list short-term exposure limits (STELs), of 5, 6, and 0.23 ppm (11.25, 13.5 and 0.5 mg/m^3), respectively the last coming from the former USSR.

The exposure assessment was based on measured data, expert judgement, on-site experience, and the EASE model (inhalation and dermal exposure assessment). Measured data on exposure levels for acrylonitrile in the mid-1970s indicated average levels of as high as 5 ppm. By the late 1980s and early 1990s, exposure levels were in the range of < 0.12 ppm to 0.49 ppm (8-h time-weighted average values, personal monitoring). Monitoring from the mid-1990s onwards indicates that average exposure levels throughout Europe for processing and production of acrylonitrile were 0.1 ppm and 0.45 ppm, respectively. Industry has confirmed that current exposure levels are significantly lower than those in earlier decades, reflecting improvements in workplace exposure control over the last decade. However for the purpose of risk characterisation a reasonable worst-case exposure level of 2 ppm (the 8-hour Occupational Exposure Limit in a number of countries) has been used for both production and further processing.

Dermal exposure to acrylonitrile during production is considered to be very unlikely under normal conditions of work as closed systems are used. Dermal exposure of workers was however considered in the risk assessment during processing of acrylonitrile to polymers including fibre production, where direct handling/contact could possibly occur. In practice, industry has confirmed that exposure by the dermal route does not occur, due to stringent use of personal protective equipment. Nevertheless, for dermal exposure a worst-case scenario was assumed i.e. between 0.0 and 0.1 mg/cm^2/day, based on EASE Modelling predictions.

The concentration of acrylonitrile in end-use products is low. Therefore, airborne exposure or dermal exposure of workers during the handling of such products will be minimal. Measured data indicate that levels of acrylonitrile in this situation are below the level of detection.

Consumer exposure

Acrylonitrile is not sold to the general public alone or as part of a preparation. Based on the identified uses in products, the main routes for potential exposure of consumers are via dermal contact/absorption through the skin, due to slow release of acrylonitrile from acrylic fibres in clothes, and via consumption/ingestion of foods packaged in acrylonitrile-derived plastics and migration of residual acrylonitrile monomer from the food packaging into food.

Residual low levels of acrylonitrile have been reported in a number of commercial polymeric materials derived from acrylonitrile. For fibres, reported levels were generally less than 1 mg/kg (1 ppm), and recent work carried out by industry indicate that current levels in both acrylic fibres and in garments derived from them are well below 1 ppm. In the risk assessment, possible migration of residual acrylonitrile from fibres was estimated with the AMEM-programme (OECD, 1993). The results indicated little potential for exposure of consumers to residual monomer in this situation. Based on the comprehensive work carried out by one major fibre producer it can be concluded that current and foreseeable users of products containing acrylonitrile-based fibres are at negligible risk from exposure to residual acrylonitrile content.

The tolerable specific migration limit is 0.02 mg acrylonitrile / kg food for food products contained in ABS plastic, as laid down by Commission Directive 90/128/EEC. If it is assumed that only 5% of human food is packaged in ABS and an average person consumes 2 kg of food and beverages/day, human intake will be no more than 2 μg/day or 0.03 μg/kg/day in the case of a bodyweight of 70 kg.

Humans exposed via the environment

Exposure of the general public via the environment is considered at two levels: (1) exposure to background levels on a regional or continental basis, and (2) exposure to potentially higher levels which may exist near industrial production and processing sites. The compartments considered for both cases are biota, drinking water and air. With respect to the regional exposure predicted results from the Mackay Level 3 model were far below those estimates calculated using EUSES. The EUSES value for Regional total daily intake for humans is calculated as $1.03 \cdot 10^{-4}$ mg/kg/day. Actual monitoring data indicate that levels of acrylonitrile are below the limits of detection in both air and drinking water, while no data were found for levels of acrylonitrile in biota.

Regarding the local case (2) the emissions data from European industry indicate that predicted local concentrations in water courses in the immediate vicinity of inland sites for production and processing of acrylonitrile range from 0-6 μg/l (background regional levels of 3 μg/l are predicted from EUSES). Higher levels were predicted in the vicinity of coastal sites without WWTP, discharging directly into the sea. However, given the continuing degradation of acrylonitrile, which is predicted to occur following initial release to local surface water and the lack of bioaccumulation potential, it is anticipated that levels of acrylonitrile in local biota will be extremely low. The assumption was made that these levels will be similar to those predicted on a regional scale by EUSES. Therefore it can be concluded that people living close to or in the vicinity of acrylonitrile production or processing plants are exposed to low to negligible levels of acrylonitrile in the air.

4.1.2 Effects assessment

Based on the results of animal studies and available human evidence, acute effects of acrylonitrile can occur following inhalation, ingestion and dermal exposure. Clinical signs resulting from acrylonitrile have been examined in a number of different animal species and have been found to vary very little between species.

Only limited data exist (specific accidents or incidents) with respect to exposure of humans. However these findings and dose levels are consistent with the information obtained from acute studies performed in animals. Based therefore mainly on the animal data, acrylonitrile is toxic by the oral, dermal and inhalation routes and causes neurotoxic effects (which relate both to acrylonitrile itself and also to the release of cyanide). Acrylonitrile should therefore be classified as "Toxic by inhalation, in contact with skin and if swallowed" (for classification, see Section 1).

Acrylonitrile is irritating to the skin and is a severe eye irritant. While there are no specific animal studies on respiratory irritancy, both short-term and long-term studies in a range of species have indicated that acrylonitrile produces irritant effects on the upper respiratory tract. As such therefore acrylonitrile should be classified as "Irritant, irritating to respiratory system and skin, risk of serious damage to eyes" (see Section 1).

Acrylonitrile is a skin sensitiser and should be classified as "Sensitising, May cause sensitisation by skin contact" (see Section 1). While there is no available data with respect to respiratory sensitisation, in practice, there are no reports of respiratory sensitisation in exposed workers. In addition, it is recognised that the control measures that have been in place for many years to protect workers against the carcinogenic effects of acrylonitrile will also protect against possible induction of sensitisation.

Studies on the toxicokinetics of acrylonitrile have shown that it is extensively absorbed and distributed after all routes of administration. Limited toxicokinetics data in humans indicate that the metabolic pathway via cyanoethylene oxide (CEO) exists in humans and generally support the conclusion that the metabolic pathways observed in experimental animals are also operative in humans. However there is further evidence that humans may possess an additional detoxification pathway, epoxide hyrolase, for CEO, which should decrease the amount of CEO leaving the liver to the systemic circulation relative to rats, where this pathway is not operative.

A large number of long-term toxicity/ carcinogenicity studies have been carried out on acrylonitrile, using the oral and inhalation routes. Both routes of exposure have been associated with lethality in a range of animal species. Target organs have been the kidney, gastrointestinal tract, central nervous system and adrenals. Neurotoxicological effects can largely be explained on the basis of release of cyanide, which may also be the ultimate causative agent in relation to the repeat dose toxicity of acrylonitrile. Local irritant effects have been observed in the respiratory tract following inhalation exposure. Human data are difficult to assess in relation to establishment of a dose-response relationship for chronic toxicity. However many of the findings in the animal repeat dose exposure studies, especially the neurological and irritation effects, reflected the reported findings in workers.

The most relevant long term toxicity/carcinogenicity study with respect to the oral route of exposure was performed by Biodynamics, in which acrylonitrile was administered orally via drinking water to 100 Fisher 344 rats/sex/group at dose levels of 1, 3, 10, 30, and 100 ppm and to a control group of 200 rats/sex. Treatment-related non-neoplastic changes were seen at 10 ppm and upwards. Mortality was increased in males at 10 ppm and in females an increase

was observed at 3 and 30 ppm. However the increase at 3 ppm was small and did not indicate a dose-response relationship. The first true indication of a dose-response relationship for mortality in females began at the 10 ppm dose level. This study was used to establish an NO(A)EL of 3 ppm (equivalent to an average daily dose of 0.25 mg/kg/day in males and 0.36 mg/kg/day in females) for the oral (drinking water) route of exposure.

In relation to the inhalation route, the Quast et al. carcinogenicity study was considered to be the key study for risk assessment purposes. Non-neoplastic changes observed in Sprague-Dawley rats exposed to 20 ppm or 80 ppm acrylonitrile for 6 hours/day, 5days/week, for 104 weeks, compromised growth retardation and early mortality in both sexes at 80 ppm and in females at 20 ppm. As a result of irritation due to acrylonitrile exposure, inflammatory and degenerative changes (hyperplasia and metaplasia of the respiratory epithelium) were present in the nasal turbinates of both exposed groups (20 and 80 ppm). A significantly increased number of rats in the 80 ppm exposure group also showed focal gliosis and perivascular cuffing in the brain. From the effects seen in this study it was concluded that the NO(A)EL is less than 20 ppm (lowest dose administered). This value of 20 ppm was considered the LO(A)EL, based on the nasal changes (local effect) which were evident at this concentration. Application of a safety factor of 5 to the level of 20 ppm to give a suggested No Adverse Effect level (NAEL) of 4 ppm was considered justifiable because of the nature of the effect (local irritancy) and the conclusion that other systemic, non-neoplastic findings in acrylonitrile-treated rats were secondary to its tumorigenic effects, rather than due to direct systemic toxicity. The conclusion is supported by the evidence from the study of Sakurai et al. (1978) that levels below 10 ppm (22.5 mg/m^3) did not cause notable irritancy.

The results of the long-term toxicity/ carcinogenicity studies indicate conclusively that acrylonitrile is carcinogenic via both the oral and inhalation routes. The animals developed tumours of the central nervous system, forestomach, intestines (including gastrointestinal tract, tongue, non-glandular stomach and small intestine), Zymbal gland (a sebaceous tissue associated with the ear duct of rodent species) and the mammary glands. While there is no doubt that acrylonitrile is an animal carcinogen the mechanism of action with respect to carcinogenicity is still relatively unclear. However as there is no definitive contrary evidence acrylonitrile must be considered to be a genotoxic carcinogen and as such it is not possible to establish a safe threshold regarding exposure to the substance. On this basis a NOEL cannot in practice be estimated or established for this particular end-point.

Acrylonitrile is weakly mutagenic in reverse mutation assays, the effect generally requiring the presence of metabolic activation. Positive results have also been obtained in mutagenicity assays using yeast and *Aspergillus* and in mammalian cell lines including mouse lymphoma cells ($TK^{+/-}$ locus and *oua* locus) and the TK6 human lymphoblast cell line. These again generally required metabolic activation (frequently only at cytotoxic concentrations). Acrylonitrile induces sister chromatid exchanges and chromosomal aberrations in *in vitro* studies, however negative responses have generally been obtained in DNA repair assays using rat hepatocytes and human epithelial cells *in vitro*. In i*n vivo* studies overall acrylonitrile appeared to be negative in a dominant lethal assay in rats, and was also negative in two mouse micronucleus studies. Conflicting results have been obtained in studies of unscheduled DNA synthesis. A number of studies in *Drosophila*, using a range of genetic markers, have given positive results.

Overall, although acrylonitrile has been shown to be weakly mutagenic in *in vitro* systems, indicative of genotoxic potential, these findings are not reliably reflected in the *in vivo* situation. This suggests that acrylonitrile or its active metabolites do not reach target tissues *in vivo*, possibly due to the detoxification of the epoxide metabolite CEO via a glutathione

conjugation pathway which may not exist in *in vitro* test systems. Nevertheless, the body of evidence presented in this report (*in vitro*), together with the positive results in *Drosophila*, leads to the conclusion that acrylonitrile must be regarded as genotoxic.

A vast amount of epidemiological data exists and various meta-analyses have considered this information. In summary, the excess risk of lung cancer from acrylonitrile exposure, if any, is small. For the less common cancers such as brain and prostate it is only possible to evaluate consistency across the available studies. When doing this a relatively imprecise estimate of risk was found for prostate and brain cancers. On the basis of the most recent studies however, there is little or no evidence to support a causal relationship between acrylonitrile exposure and cancer in man. From the results of the animals studies acrylonitrile is an animal carcinogen and the current classification as a Category 2 carcinogen is appropriate (see Section 1). However based on the evidence presented, in particular the epidemiological information available, while acrylonitrile is an animal carcinogen the risk to humans is low considering current exposure in the workplace and the lack of association arising from the large cohort studies performed.

The results of a 3-generation reproduction study did not show any effects on fertility, although effects were seen on pup viability and bodyweights of pups in all 3 generations at 21 days were also reduced. These effects could be attributed to maternal toxicity. A number of other studies have also indicated that acrylonitrile is foetoxic, as evidenced by dose-dependent reductions in pup weight at exposure levels which are also maternally toxic. A No Effect Level of 12 ppm for the foetotoxic effect was established. While effects on the testis in mice and rats have been reported by some authors in short term studies, this may have been a secondary effect associated with systemic toxicity. However, testicular toxicity has not been reported in a 2-year inhalation study in rats at 80 ppm (equivalent oral uptake 17 mg/kg/day) or in a 90-day oral gavage study in mice at a top dose of 12 mg/kg/day. There are no data on fertility in humans.

It can be concluded that existing animal data do not show any clear indication of fertility, dominant lethal, reproductive or teratogenic effects of acrylonitrile at doses below those producing parental toxicity. Classification as toxic for reproduction is not considered appropriate given the maternal toxicity seen, the confounding influence of disease and the negative outcome of the 1993 developmental study where previously mated rats were exposed to dose levels of 0, 12, 25, 50 and 100 ppm acrylonitrile by inhalation 6 hr/day from day 6-20 of gestation.

4.1.3 Risk characterisation

Workers

Exposure of humans to acrylonitrile is possible in the workplace, during production of acrylonitrile and its use in the manufacture of acrylic fibres, ABS-SAN plastics, nitrile rubbers, other intermediates such as acrylamide and adiponitrile and other end uses.

Conclusion (iii) is reached in relation to the following end points: (1) repeated dose (systemic) toxicity, (2) carcinogenicity.

In relation to conclusion (iii) for repeated dose (systemic) toxicity by the inhalation and by route-to-route extrapolation, the dermal route, this primarily reflects the toxicity seen in

chronic studies in rats and the relatively low Margins of Safety (MOSs) between anticipated exposure levels and doses producing toxicity. Many of the findings in the animal repeated dose studies are mirrored in reported findings in workers. Overall, however, the human data are difficult to assess in relation to establishment of a dose-response relationship. The EU Working Group on Classification and Labelling agreed that acrylonitrile should not be classified with R 48 (risk of serious damage to health on prolonged exposure) based on the information available. Nevertheless, for the purposes of this risk assessment, given the difficulties in assessing the human data and the low MOSs achieved, it is recommended that conclusion (iii) be applied to the repeated dose (systemic) toxicity end point. It is however acknowledged that strict controls on exposure to acrylonitrile apply in the industry for this classified carcinogen, and industry confirm that exposure levels in the workplace are much less than 2 ppm. For example in the 1990s, in production and processing sectors, the levels achieved were less than 1 ppm and 0.1-1 ppm, respectively.

In relation to conclusion (iii) for carcinogenicity, it is accepted that there is a risk at any level of exposure, given that acrylonitrile is currently regarded as a carcinogen for which a threshold cannot be reliably identified. The magnitude of this risk has been estimated to lie between $1.3 \cdot 10^{-4}$ to $1.8 \cdot 10^{-2}$ for workers exposed to 2 ppm (the current OEL in a number of EU countries) for 8 hours a day, 5 days a week and a working life of 40 years. A Margin of Exposure (MOE) of 57.5 has been derived, based on a T_{25} of 16.1 mg/kg/day in the male rat obtained from the Quast 2-year inhalation study.

Conclusion (ii) is reached for the end points of acute toxicity, skin, eye and respiratory irritancy, skin sensitisation, corrosivity, repeated dose (local) toxicity by the inhalation route, neurotoxicity, mutagenicity and reproductive toxicity.

Consumers

There is no exposure of consumers directly to acrylonitrile. However there is potential for indirect exposure of consumers as a consequence of use of products manufactured from acrylonitrile, due to the presence of residual monomer. Risk characterisation for the endpoints of acute toxicity, irritation and corrosivity is not necessary given that consumers will never come in contact with acrylonitrile liquid. The relevant endpoints therefore are skin sensitisation, repeat dose toxicity, carcinogenicity, mutagenicity and reproductive toxicity.

Conclusion (iii) is reached for the end point carcinogenicity.

Regarding the level of carcinogenic risk for consumers related to inhalation of acrylonitrile, a life time exposure scenario where a 70 kg man inhales 20 m^3 of air a day, containing 1 part per trillion acrylonitrile a risk estimate of $3.3 \cdot 10^{-8}$ was derived. More recently this database was re-evaluated using the EPA's cancer risk assessment guidelines giving a risk estimate of between $8.2 \cdot 10^{-6}$ to $1.1 \cdot 10^{-5}$ associated with lifetime continuous exposure to 1 $\mu g/m^3$ ($0.44 \cdot 10^{-3}$ ppm). In addition the Committee on Carcinogenicity of Chemicals in Food (UK) and the Food Additives and Contamination Committee (UK) considered the levels of contamination with acrylonitrile monomer to be very low and that the general public were not at a measurable risk from exposure to acrylonitrile.

However, acrylonitrile is a carcinogen for which a threshold cannot be reliably identified; therefore it is considered that **conclusion (iii)** is appropriate, since risks cannot be excluded for all exposure scenarios. However, since the predicted exposures are very low, the risks will

be already very low, and this should be taken into account when considering the adequacy of controls feasibility and practicability of further specific risk reduction measures.

Conclusion (ii) is reached for the end points of skin sensitisation, repeated dose toxicity by the inhalation or (by route-to-route extrapolation) the dermal route, mutagenicity and reproductive toxicity, based on the calculated reasonable worst-case exposure levels and the margins of safety achieved.

Humans exposed via the environment

Indirect exposure of the general public via the environment from consumption of biota or drinking water and exposure to air containing residual acrylonitrile is theoretically possible although considered to be of low risk due to the extremely low levels calculated or derived from actual monitoring data. Assessment of exposure via this route identified two populations for consideration i.e. (1) populations exposed to background levels on a regional or continental basis and (2) populations exposed to potentially higher levels which could conceivably be found near industrial production and processing sites.

While acrylonitrile is acutely toxic, irritant and sensitising, it is considered that there is no concern for populations in either category (1) or category (2) in relation to these hazards, by any route of exposure, given the very low levels of exposure anticipated: **conclusion (ii)**.

In relation to mutagenicity, reflecting the absence of *in vivo* mutagenicity, the rapid detoxification of the mutagenic metabolite CEO in human by epoxide hydrolase and the fact that acrylonitrile is not classified as mutagenic, acrylonitrile is of no concern for this end point: **conclusion (ii)**.

The endpoint of concern remaining is carcinogenicity. There could be some concern for carcinogenicity for humans exposed via air, with respect to the immediate vicinity of plants (**conclusion (iii)**), based mainly on potential for local exposure to a carcinogen for which a threshold cannot be reliably identified. This conclusion however should be qualified indicating that risks are already very low. This should be taken into account when considering the adequacy of controls feasibility and practicability of further specific risk reduction measures.

4.2 HUMAN HEALTH (PHYSICO-CHEMICAL PROPERTIES)

Assessment of physico-chemical hazards has indicated that acrylonitrile is highly flammable and has explosive properties when mixed with air in certain proportions. Spontaneous exothermic polymerisation of acrylonitrile also presents a risk of explosion. The use of closed systems and stringent safety controls indicates that the potential risk to workers is minimal under conditions of normal handling and use: **conclusion (ii)**.

In relation to consumers, given the very low levels of free (un-reacted) monomer to which they are likely to be exposed, it is concluded that acrylonitrile is unlikely to present a risk to this population due to physico-chemical hazards: **conclusion (ii)**.

5 RESULTS

5.1 ENVIRONMENT

Aquatic compartment (incl. sediment)

Conclusion (iii) There is a need for limiting the risks; risk reduction measures which are already being applied shall be taken into account.

This conclusion is reached because of concerns for effects on the local aquatic sphere (including sediment) as a consequence of exposure arising from production of acrylic fibres at a particular site.

Conclusion (ii) There is at present no need for further information or testing or risk reduction measures beyond those which are being applied already.

This conclusion applies to the aquatic compartment including sediment and microorganisms, for production of acrylonitrile and further processing to fibres and other plastics, with the exception of processing to acrylic fibres at one site only.

It also applies to the terrestrial compartment, atmospheric compartment and secondary poisoning, for production of acrylonitrile and further processing to fibres and other plastics.

5.2 HUMAN HEALTH

5.2.1 Human health (toxicity)

Workers

Conclusion (iii) There is a need for limiting the risks; risk reduction measures which are already being applied shall be taken into account.

This conclusion is reached because of concerns for general systemic effects and carcinogenicity as a consequence of exposure arising during the production and processing of the substance.

Conclusion (ii) There is at present no need for further information or testing or risk reduction measures beyond those which are being applied already.

This conclusion applies to the end points of acute toxicity, skin, eye and respiratory irritancy, skin sensitisation, corrosivity, repeated dose (local) toxicity by the inhalation route, neurotoxicity, mutagenicity and reproductive toxicity.

Consumers

Conclusion (iii) There is a need for limiting the risks; risk reduction measures which are already being applied shall be taken into account.

This conclusion is reached because of concerns for carcinogenicity.

Risks cannot be excluded for all exposure scenarios, as the substance is identified as a non-threshold carcinogen. The adequacy of existing controls and the feasibility and practicability of

further specific measures should be considered. However, the risk assessment indicates that risks are already low. This should be taken into account when considering the adequacy of existing controls and the feasibility and practicability of further specific risk reduction measures.

Conclusion (ii) There is at present no need for further information or testing or risk reduction measures beyond those which are being applied already.

This conclusion applies to the end points of skin sensitisation, repeated dose toxicity by the inhalation or (by route-to-route extrapolation) the dermal route, mutagenicity and reproductive toxicity.

Humans exposed via the environment

Conclusion (iii) There is a need for limiting the risks; risk reduction measures which are already being applied shall be taken into account.

This conclusion is reached because of concerns for carcinogenicity after highest predicted atmosphere concentrations at a local level.

There could be some concern for carcinogenicity for humans exposed via air, with respect to the immediate vicinity of plants, based mainly on potential for local exposure to a carcinogen for which a threshold cannot be reliably identified. This conclusion however should be qualified indicating that risks are already very low. This should be taken into account when considering the adequacy of controls feasibility and practicability of further specific risk reduction measures.

Conclusion (ii) There is at present no need for further information or testing or risk reduction measures beyond those which are being applied already.

This conclusion applies to all other endpoints.

5.2.2 Human health (risks from physico-chemical properties)

Conclusion (ii) There is at present no need for further information and/or testing or for risk reduction measures beyond those which are being applied already.

This conclusion is reached because the risk assessment shows that risks to workers, consumers and humans exposed via the environment related to physico-chemical properties are not expected. Risk reduction measures already being applied are considered sufficient.

Appendix A Local PEC and other emission parameters for surface water for acrylonitrile production plants in Europe

Table A.1 Local PEC and other emission parameters for surface water for acrylonitrile production plants in Europe

In this and subsequent PEC tables, some values are based on detection limits. Thus their PEC is a 'less than' value.

Site	Production t/y	Released t/y	Daily release t/d	WWTP	C, influent mg/l	C effluent mg/l *	Discharge to	Dilution factor	C, water mg/l	C water an mg/l	PEC, wate mg/l	PEC wat.a mg/l	RCR water	PEC, sed mg/kg	RCRstp	RCR sed
1	***120500***	***0.100***	0.0003	Yes	0.167	**0.1000**	***sea***	10	0.010000	0.00822	0.0128	0.0110	0.754	0.01058	0.0200	0.8399
2 (+BB)	***190000***	***4.000***	0.0133	Yes	***3.800***	***0.0013***	***river***	***30***	0.000043	0.00004	0.0029	0.0028	0.168	0.00236	0.0003	0.1871
3	***85000***	***0.043***	0.0001	Yes	***2.500***	0.0036	***sea***	10	0.000363	0.00030	0.0032	0.0031	0.187	0.00262	0.0007	0.2080
4 (+D+EE)	***300000***	***0.031***	0.0001	Yes	0.052	***0.0020***	***river***	**1529**	0.000001	0.00000	0.0028	0.0028	0.165	0.00232	0.0004	0.1843
5	***280000***	***9.300***	0.0310	No	15.500	***5.8000***	***estuary***	***500***	0.011600	0.00953	0.0144	0.0123	0.848	0.01190	n.a.	0.9448
6	***60000***	***0.040***	0.0001	Yes	0.067	***0.3700***	***river***	***2000***	0.000185	0.00015	0.0030	0.0030	0.176	0.00247	0.0740	0.1964
7	***110000***	***0.024***	0.0001	Yes	0.040	***0.0500***	***river***	**4154**	0.000012	0.00001	0.0028	0.0028	0.166	0.00233	0.0100	0.1850
8	***105000***	***0.053***	0.0002	Yes	***2.500***	0.0044	***sea***	10	0.000439	0.00036	0.0032	0.0032	0.191	0.00268	0.0009	0.2130
Total	1250500	13.59														

Note Numbers in bold italics actual figures
Where a production facility and further processing facility(s) are located at the same site, the production figure in column 2 is for the production site only, but emissions relate to all facilities at the site (as in 4 (+D+EE)
Production figures rounded to nearest 100.
Where an influent concentration was lower than an effluent concentration calculated, the influent was used as the effluent concentration
p.a.release / 300 = daily release t/d
[Daily release (t/d) / STP volume (default 2,000,000 l/d)] x 1,000,000,000 (convert t to mg) = C, influent mg/l
C, effluent = C, influent * fraction to water (EUSES 0.116). This accounts for fraction of 0.85 being degraded, 0.0324 discharged to air, and a fraction of 0.00132 in sludge.
Note that the fraction effluent degraded in STP of 0.885 is from EUSES for readily biodegradable, as agreed for industrial sites with WWTP, but does not apply to site 5
However, it was only necessary to apply these fractions for sites which had not provided effluent concentrations.
For sites 3 and 8, C, effluent = C, influent/80*0.116 and C, influent/66*0.116 respectively, since the acrylonitrile waste stream is further diluted by other aqueous waste (240 m3 in 19.200 m3 and 360 m3 in 24,000 m3 respectively) before discharge into WWTP
C, effluent / dilution factor (default 10) = C, water.
Where a site discharges to an estuary the dilution factor has been derived from the main river flow into the estuary only.
Where additional dilution data has been available for WWTP this has been used in calculating effluent concentrations.
C water + PEC regional = PEC water (PEC regional (EUSES) = 0.00281)
PEC water, annual = C, water annual + PEC regional (PEC regional (EUSES) = 0.00281)
C water * 300/365 = C, water annual
RCR = PEC/PNEC
PNEC surfacewater = 0.017 where NOEC / 10
* C local effluent = PEC STP
RCR stp = PEC stp / PNEC where PNEC = 5 mg/l
PEC sediment = (0.95/1150)*1000*PECwater = 0.8260869 * PECwater
PNEC sediment = 0.0126 mg/kg (Section 3.2.1.4)

Appendix B Local PEC and other emission parameters for surface water for acrylonitrile processing plants in Europe

Table B.1 Local PEC and other emission parameters for surface water for acrylonitrile processing plants in Europe

Site	Processing capacity t/y	Process releases t/y	Daily release t/d	C, influent mg/l	WWTP	C,effluent mg/l	Dilution factor		C, water mg/l	C water. annual mg/l	PEC, water mg/l	PECwater annual mg/l	RCR water	PEC, sed mg/kg	RCR stp	RCR sed
Fibre																
B (scenario 2)	***70000***	***5.750***	0.0192	9.583	No	***7.200***	***1123***	***2nd river***	0.0064	0.005	0.0092	0.0081	0.54	0.0076	n.a.	0.60
C (scenario 2)	***40000***	***0.200***	0.0007	0.333	No	***0.200***	***38681***	***estuary***	0.0000	0.000	0.0028	0.0028	0.17	0.0023	n.a.	0.18
D (+EE+4)	***112000***	***0.031***	0.0001	0.052	Yes	***0.002***	***1529***	***river***	0.0000	0.000	0.0028	0.0028	0.17	0.0023	0.00	0.18
E	***78000***	***294.000***	0.9800	490.000	No	***35.000***	***701***	***estuary***	0.0499	0.041	0.0527	0.0438	3.10	0.0436	n.a.	3.46
F	***130000***	***0.235***	0.0008	***35.000***	Yes	***0.250***	***2000***		0.0001	0.000	0.0029	0.0029	0.17	0.0024	0.05	0.19
G	***62000***	***0.200***	0.0007	***80.000***	Yes	***0.100***	***20***		0.0050	0.004	0.0078	0.0069	0.46	0.0065	0.02	0.51
H	***40000***	***2.134***	0.0071	3.557	Yes	***0.500***	***100***		0.0050	0.004	0.0078	0.0069	0.46	0.0065	0.10	0.51
J	***49000***	***0.008***	0.0000	0.013	Yes	0.002	10		0.0002	0.000	0.0030	0.0029	0.17	0.0024	0.00	0.19
K	***78000***	***0.350***	0.0012	***10.000***	Yes	***0.250***	***59***		0.0042	0.003	0.0070	0.0063	0.41	0.0058	0.05	0.46
Total	659000	302.908														
ABS/SAN																
AA	***10300***	***3.600***	0.0120	6.000	No	***1.160***	***1400***	***estuary***	0.0008	0.001	0.0036	0.0035	0.21	0.0030	n.a.	0.24
BB (+2)	***26000***	***4.000***	0.0133	***3.800***	Yes	***0.001***	***30***		0.0000	0.000	0.0028	0.0028	0.17	0.0023	0.00	0.19
CC	***18000***	***9.000***	0.0300	***0.500***	Yes	0.058	10		0.0058	0.005	0.0086	0.0076	0.51	0.0071	0.01	0.56
DD	***5000***	***0.500***	0.0017	0.833	Yes	***0.100***	***151***		0.0007	0.001	0.0035	0.0034	0.20	0.0029	0.02	0.23
EE (+D+4)	***30000***	***0.031***	0.0001	0.052	Yes	***0.002***	**1529**		0.0000	0.000	0.0028	0.0028	0.17	0.0023	0.00	0.18
FF	***4000***	***0.500***	0.0017	0.833	No	0.833	***7213***	***river***	0.0001	0.000	0.0029	0.0029	0.17	0.0024	0.17	0.15
GG	***16000***	***0.004***	0.0000	0.007	Yes	***0.009***	***573***	***estuary***	0.0000	0.000	0.0028	0.0028	0.17	0.0023	0.00	0.19
HH	***25000***	***0.004***	0.0000	0.007	Yes	***0.001***	***818***		0.0000	0.000	0.0028	0.0028	0.17	0.0023	0.00	0.18
II	***27000***	***0.010***	0.0000	0.017	Yes	0.002	10		0.0002	0.000	0.0030	0.0030	0.18	0.0025	0.00	0.16
JJ	***12000***	***0.000***	0.0000	0.000	Yes	0.000	10	***sea***	0.0000	0.000	0.0028	0.0028	0.17	0.0023	0.00	0.18
KK	***4500***	***5.720***	0.0191	***6.200***	Yes	0.032	10	***sea***	0.0032	0.003	0.0060	0.0054	0.35	0.0050	0.01	0.39
LL (+HHH)	***48000***	***13.200***	0.0440	22.000	Yes	***0.050***	***156***		0.0003	0.000	0.0031	0.0031	0.18	0.0026	0.01	0.21
MM	***16000***	***0.100***	0.0003	0.167	Yes	***0.050***	***125***		0.0004	0.000	0.0032	0.0031	0.19	0.0027	0.01	0.21
Total	241800	36.669														

Table B.1 continued overleaf

Table B.1 continued Local PEC and other emission parameters for surface water for acrylonitrile processing plants in Europe

Site	Processing capacity t/y	Processing release t/y	Daily release t/d	C, influent mg/l	WWTP	C,effluent mg/l	Dilution factor		C, water mg/l	C water annual mg/l	PEC, water mg/l	PECwater annual mg/l	RCR water	PEC, sed mg/kg	RCR stp	RCR sed
NB COPOLYMERS																
AAA	***4500***	***8.139***	0.0271	13.565	No	***11.760***	1250	***sea***	0.0094	0.008	0.0122	0.0105	0.72	0.0101	n.a.	0.80
BBB	***1200***	***5.260***	0.0175	***50.000***	Yes	5.800	***24570***		0.0002	0.000	0.0030	0.0030	0.18	0.0025	1.16	0.20
CCC	***1100***	***0.028***	0.0001	0.047	Yes	0.005	10		0.0005	0.000	0.0034	0.0033	0.20	0.0028	0.00	0.22
DDD	***1500***	***0.090***	0.0003	0.150	Yes	***0.018***	10		0.0018	0.001	0.0046	0.0043	0.27	0.0038	0.00	0.30
EEE	***10450***	***3.150***	0.0105	5.250	No	5.250	***14800***		0.0004	0.000	0.0032	0.0031	0.19	0.0026	n.a.	0.21
FFF	***12000***	***2.700***	0.0090	4.500	Yes	***0.050***	10		0.0050	0.004	0.0078	0.0069	0.46	0.0065	0.01	0.51
GGG	***4400***	***3.200***	0.0107	5.333	Yes	***0.050***	10	***sea***	0.0050	0.004	0.0078	0.0069	0.46	0.0065	0.01	0.51
HHH (+LL)	***600***	***13.200***	0.0440	22.000	Yes	***0.100***	***156***		0.0006	0.001	0.0035	0.0033	0.20	0.0029	0.02	0.23
JJJ	***10000***	***4.000***	0.0133	***2.480***	Yes	0.008	10		0.0008	0.001	0.0036	0.0035	0.21	0.0030	0.00	0.24
Total	45750	39.767														
ACRYLAMIDE + ADIPONITRILE																
L	***39000***	***0.000***	0.0000	0.000	Yes	0.000	10		0.0000	0.000	0.0028	0.0028	0.17	0.0023	0.00	0.18
M	***40000***	***0.030***	0.0001	***1.000***	Yes	***0.100***	***150000***	***river***	0.0000	0.000	0.0028	0.0028	0.17	0.0023	0.02	0.18
N	***161000***	***0.000***	0.0000	0.000	Yes	0.000	***500***	***estuary***	0.0000	0.000	0.0028	0.0028	0.17	0.0023	0.00	0.18
O	***23000***	***0.000***	0.0000	0.000	Yes	0.000	10		0.0000	0.000	0.0028	0.0028	0.17	0.0023	0.00	0.18
Total	263000	0.030														

Where a production facility and further processing facility(s) are located at the same site, the production figure in column 2 is for the processing site only, but emissions relate to all facilities at the site (as in 4 (+D+EE)

p.a.release / 300 = daily release t/d

[Daily release (t/d) / STP volume (default 2,000,000 l/d)] x 1,000,000,000 (convert t to mg) = C, influent mg/l

C, effluent = C, influent * fraction to water (EUSES 0.116). This accounts for fraction of 0.85 being degraded, 0.0324 discharged to air, and a fraction of 0.00132 in sludge. Note that the fraction effluent degraded in STP of 0.85 is from EUSES for 'ready biodegradable'.

For site KK, C, effluent = C, influent/22.5*0.116, since the acrylonitrile waste stream is further diluted by other aqueous waste (40 m3 in 900 m3) before discharge into WWTP.

For site JJJ, C, effluent = C, influent/35*0.116, for the same reason as cited for site KK

The fraction to water (less that lost to air and sludge) has only been applied to sites which have been reported to have an STP.

For other sites the C, effluent = C influent.

It was only necessary to apply these fractions to sites which had not provided actual effluent concentrations.

C, effluent / dilution factor (default 10) = C, water.

C water + PEC regional = PEC water (PEC regional (EUSES) = 0.0028)
C water * 300/365 = C, water annual

RCR = PEC/PNEC PNECwater = 0.017

PEC sediment = (0.95/1150)*1000*PECwater = 0.8260869 * PECwater

PNEC sediment = 0.0126 (Section 3.2.1.4)
Site B, Scenario 2 = discharge to main river via 100 m canal
Site C, Scenario 2 = dilution factor proposed by industry

Appendix C Local PEC and other emission parameters to air for acrylonitrile production plants in Europe

Table C.1 Local PEC and other emission parameters to air for acrylonitrile production plants in Europe

Site	Production t / y	Released t/y	Daily relea t/d	E,air Kg/d	E,effluent mg/l	E air STP kg/d	C, air mg/m3	C air ann. mg/m3	PEC, air mg/m3	PECair,anr mg/m3	RCR air
1	***120500***	***1.235***	0.004	4.12	***0.1000***	0.0032	0.0011	0.001	0.001	0.001	0.002
2 (+BB)	***190000***	***12.400***	0.041	***99.00***	***0.0013***	0.0000	***0.0006***	0.000	0.001	0.001	0.001
3	***85000***	***5.000***	0.017	16.67	0.0036	0.0001	0.0046	0.004	0.005	0.005	0.009
4 (+D+EE)	***300000***	***3.200***	0.011	10.67	***0.0020***	0.0001	0.0030	0.002	0.003	0.003	0.006
5	***280000***	***259.000***	0.863	863.33	***5.8000***	n.a.	0.2400	0.197	0.240	0.240	0.480
6	***60000***	***0.054***	0.000	0.18	***0.3700***	0.0120	0.0001	0.000	0.000	0.000	0.000
7	***110000***	***2.300***	0.008	7.67	***0.0500***	0.0016	0.0021	0.002	0.002	0.002	0.004
8	***105000***	***2.000***	0.007	6.67	0.0044	0.0001	0.0019	0.002	0.002	0.002	0.004
Total	1250500	283									

Note Numbers in bold italics are figures provided by industry (emissions provided for all sites)
Where a production facility and further processing facility(s) are located at the same site, the production figure in column 2 is for the production site only, but emissions relate to all facilities at the site (as in 4(+D+EE)
n.a. = not applicable
p.a.release / 300 = daily release t/d
Indirect emission to air from STP (EUSES) as fraction of effluent = 0.0324.
This only applies to sites with an STP, i.e. sites 1, 2, 3, 4, 6, 7 and 8.
C air = (direct + indirect emissions to air)* 0.000278 (from TGD)
C air + PEC regional = PEC air
PEC regional (EUSES) = 0.0000708 mg/m3
C air * 300/365 = C air, annual
RCR = PEC/PNEC, where PNEC = 0.5 mg/m3
The total release for site 5 represent 62 tonnes from production (monitored) and 197 tonnes from storage (modelled)

Appendix D Local PEC and other emission parameters to air for acrylonitrile processing plants in Europe

Table D.1 Local PEC and other emission parameters to air for acrylonitrile processing plants in Europe

Site	Processing	Released	Daily releas	E a	E, effluent	E air STP	C, air	C air ann	PEC, air	PEC air, ani	RCR
	t / y	t/y	t/d	Kg/d	mg/l	Kg/d	mg/m3	mg/m3	mg/m3	mg/m3	air
FIBRES											
B	***70000***	***14.000***	0.047	46.67	***7.200***	n.a.	0.013	0.011	0.0130	0.0107	0.0261
C	***40000***	***20.400***	0.068	68.00	***0.200***	n.a.	0.019	0.016	0.0190	0.0156	0.0379
D (+EE+4)	***112000***	***0.085***	0.000	0.28	***0.002***	0.0001	0.000	0.000	0.0001	0.0001	0.0003
E	***78000***	***154.000***	0.513	513.33	***35.000***	n.a.	0.143	0.117	0.1428	0.1174	0.2856
F	***130000***	***26.200***	0.087	87.33	***0.250***	0.0081	0.024	0.020	0.0244	0.0200	0.0487
G	***62000***	***5.000***	0.017	16.67	***0.100***	0.0032	0.005	0.004	0.0047	0.0039	0.0094
H	***40000***	***41.175***	0.137	137.25	***0.500***	0.0162	0.038	0.031	0.0382	0.0314	0.0765
J	***49000***	***13.300***	0.044	44.33	0.002	0.0001	0.012	0.010	0.0124	0.0102	0.0248
K	***78000***	***16.000***	0.053	53.33	***0.250***	0.0081	0.015	0.012	0.0149	0.0123	0.0298
Total	***659000***	***290.160***									
ABS/SAN											
AA	***10300***	***35.000***	0.117	116.67	***1.160***	n.a.	0.032	0.027	0.0325	0.0267	0.0650
BB (+2)	***26000***	***23.500***	0.078	***99.00***	***0.001***	0.0000	***0.0006***	0.000	0.0007	0.0006	0.0013
CC	***18000***	***1.000***	0.003	3.33	0.058	0.0019	0.001	0.001	0.0010	0.0008	0.0020
DD	***5000***	***3.000***	0.010	10.00	***0.100***	0.0032	0.003	0.002	0.0029	0.0024	0.0057
EE (+D+4)	***30000***	***3.100***	0.010	10.33	***0.002***	0.0001	0.003	0.002	0.0029	0.0024	0.0059
FF	***4000***	***4.300***	0.014	14.33	0.833	n.a.	0.004	0.003	0.0041	0.0033	0.0081
GG	***16000***	***73***	0.243	243.0	***0.009***	0.0003	0.068	0.056	0.0676	0.056	0.13525
HH	***25000***	***1.450***	0.005	4.83	***0.001***	0.0000	0.001	0.056	0.0014	0.0556	0.0028
II	***27000***	***0.585***	0.002	1.95	0.002	0.0001	0.001	0.000	0.0006	0.0005	0.0012
JJ	***12000***	***17.000***	0.057	56.67	***0.000***	0.0000	0.016	0.013	0.0158	0.0130	0.0316
KK	***4500***	***11.000***	0.037	36.67	0.032	0.0010	0.010	0.008	0.0103	0.0085	0.0205
LL (+HHH)	***48000***	***5.500***	0.018	18.33	***0.050***	0.0016	0.005	0.004	0.0052	0.0043	0.0103
MM	***16000***	***0.000***	0.000	0.00	***0.050***	0.0016	0.000	0.000	0.0001	0.0001	0.0001
Total	***241800***	***178.435***									

Notes on Appendix 1.4 are provided on the following page

Table D.1 continued overleaf

Table D.1 continued Local PEC and other emission parameters to air for acrylonitrile processing plants in Europe

AAA	***4500***	***21.600***	0.072	72.00	***11.760***	n.a.	0.020	0.016	0.0201	0.0165	0.0402
BBB	***1200***	***0.018***	0.000	0.06	5.850	0.1895	0.000	0.000	0.0001	0.0001	0.0003
CCC	***1100***	***0.005***	0.000	0.02	0.005	0.0002	0.000	0.000	0.0001	0.0001	0.0002
DDD	***1500***	***1.000***	0.003	3.33	***0.018***	0.0006	0.001	0.001	0.0010	0.0008	0.0020
EEE	***10450***	***0.600***	0.002	2.00	5.250	n.a.	0.001	0.000	0.0006	0.0005	0.0013
FFF	***12000***	***1.100***	0.004	3.67	***0.050***	0.0016	0.001	0.001	0.0011	0.0009	0.0022
GGG	***4400***	***20.200***	0.067	67.33	0.050	0.0016	0.019	0.015	0.0188	0.0155	0.0376
HHH (+LL)	***600***	***5.500***	0.018	18.33	***0.100***	0.0032	0.005	0.004	0.0052	0.0043	0.0103
JJJ	***10000***	***4.000***	0.013	13.33	0.008	0.0003	0.004	0.003	0.0038	0.0031	0.0076
Total	***45750***	***54.023***									
ACRYLAMIDE + ADIPONITRILE											
L	***39000***	***4.500***	0.015	15.00	***0.000***	0.0000	0.004	0.003	0.0042	0.0035	0.0085
M	***40000***	***1.500***	0.005	5.00	***0.100***	0.0032	0.001	0.001	0.0015	0.0012	0.0029
N	***161000***	***95.000***	0.317	316.67	***0.000***	0.0000	0.088	0.072	0.0881	0.0724	0.1762
O	***23000***	***0.053***	0.000	0.18	***0.000***	0.0000	0.000	0.000	0.0001	0.0001	0.0002
Total	263000	101.053									

Note Numbers in bold italics are figures provided by industry (emissions were provided for all sites)
Where a production facility and further processing facility(s) are located at the same site, the production figure in column 2 is for the processing site only, but emissions relate to all facilities at the site (as in D (+4+EE)
p.a.release / 300 = daily release t/d
Indirect emission to air from STP (EUSES) = fraction 0.0324.
This only applies to sites with STP; i.e. D, F, G, H, J, K, BB, CC, DD, EE, GG, HH, II, JJ, KK, LL, MM, BBB,CCC, DDD, FFF, GGG, HHH, JJJ, K, M, N, O.
C air = (direct + indirect emissions to air)* 0.000278 (from TGD)
C air + PEC regional = PEC air
PEC regional (EUSES) = 0.0000709 mg/m3
The total release for site N represent 62 tonnes from production (monitored) and 54 tonnes from storage (modelled)