

Letter report 601782015/2009 R. van Herwijnen

# Environmental risk limits for acrylonitrile



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This investigation has been performed by order and for the account of Directorate-General for Environmental Protection, Directorate Environmental Safety and Risk Management, within the framework of 'International and National Environmental Quality Standards for Substances in the Netherlands' (INS).

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# Acknowledgements

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### Rapport in het kort

#### Milieurisicogrenzen voor acrylonitril

Dit rapport geeft milieurisicogrenzen voor acrylonitril in (grond)water, bodem en lucht. Milieurisicogrenzen zijn de technisch-wetenschappelijke advieswaarden voor de uiteindelijke milieukwaliteitsnormen in Nederland. De milieurisicogrenzen voor acrylonitril zijn gebaseerd op de uitkomsten van de EU risicobeoordeling voor acrylonitril (Bestaande Stoffen Verordening 793/93). De afleiding van de milieurisicogrenzen sluit tevens aan bij de richtlijnen uit de Kaderrichtlijn Water. Omdat er geen monitoringsgegevens beschikbaar zijn kan geen verwachting worden uitgesproken of de afgeleide milieurisicogrenzen overschreden zullen worden.

Trefwoorden: milieukwaliteitsnormen; milieurisicogrenzen; acrylonitril; maximaal toelaatbaar risiconiveau; verwaarloosbaar risiconiveau

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### **Summary**

Environmental risk limits (ERLs) are derived using ecotoxicological, physico-chemical and human toxicological data. They represent environmental concentrations of a substance offering different levels of protection to man and ecosystems. It should be noted that the ERLs are scientifically derived values. They serve as advisory values for the Dutch Steering Committee for Substances, which is appointed to set the Environmental Quality Standards (EQSs) from these ERLs. ERLs should thus be considered as preliminary values that do not have any official status.

This report contains ERLs for acrylonitrile in water, groundwater, soil and air. The following ERLs are derived: negligible concentration (NC), maximum permissible concentration (MPC), maximum acceptable concentration for ecosystems (MAC $_{eco}$ ), and serious risk concentration for ecosystems (SRC $_{eco}$ ). The risk limits were solely based on data presented in the Risk Assessment Report (RAR) for this compound, prepared under the European Existing Substances Regulation (793/93/EEC). No risk limits were derived for the sediment compartment, because of the relatively low sediment-water partition coefficient. The substance has a very high vapour pressure but the high water solubility and moderate Henry coefficient make exposure though the water compartment not unrealistic.

For the derivation of the MPC and  $MAC_{eco}$  for water, the methodology used is in accordance with the Water Framework Directive. This methodology is based on the Technical Guidance Document on risk assessment for new and existing substances and biocides (European Commission (Joint Research Centre), 2003). For the NC and the  $SRC_{eco}$ , the guidance developed for the project 'International and National Environmental Quality Standards for Substances in the Netherlands' was used (Van Vlaardingen and Verbruggen, 2007). An overview of the derived environmental risk limits is given in Table 1.

Monitoring data for acrylonitrile in the Dutch environment are not available. Therefore it cannot be judged if the derived ERLs are being exceeded.

Table 1. Derived MPC, NC, MAC<sub>eco</sub>, and SRC<sub>eco</sub> values for acrylonitrile.

ERL	unit	value			
		MPC	NC	$MAC_{eco}$	$SRC_{eco}$
water <sup>a</sup>	ng.L <sup>-1</sup>	36	0.36	$1.7 \times 10^4$	$1.3 \times 10^6$
drinking water b	ng.L <sup>-1</sup>	98			
marine	ng.L <sup>-1</sup>	36	0.36	$1.7 \times 10^3$	$1.3 \times 10^6$
sediment	μg.kg <sub>dwt</sub> -1	n.d.			
soil <sup>c</sup>	μg.kg <sub>dwt</sub> -1	0.66	$6.6 \times 10^{-3}$		$1.5 \times 10^3$
groundwater	μg.kg <sub>dwt</sub> -1 μg.kg <sub>dwt</sub> -1 ng.L <sup>-1</sup>	98	0.98		$1.3 \times 10^6$
air	ng.m <sup>-3</sup>	90	0.90		

<sup>&</sup>lt;sup>a</sup> From the MPC<sub>eco, water</sub>, MPC<sub>sp, water</sub> and MPC<sub>hh, food, water</sub> the lowest one is selected as the 'overall' MPC<sub>water</sub>.

<sup>&</sup>lt;sup>b</sup> The exact way of implementation of the  $MPC_{dw, water}$  in the Netherlands is at present under discussion. Therefore, the  $MPC_{dw, water}$  is presented as a separate value in this report.

<sup>&</sup>lt;sup>c</sup> Expressed on the basis of Dutch standard soil.

n.d. = not derived.

### 1 Introduction

### 1.1 Project framework

In this report environmental risk limits (ERLs) for surface water (freshwater and marine), groundwater, soil and air are derived for acrylonitrile. The following ERLs are considered:

- Negligible Concentration (NC) concentration at which effects to ecosystems are expected to be negligible and functional properties of ecosystems must be safeguarded fully. It defines a safety margin which should exclude combination toxicity. The NC is derived by dividing the MPC (see next bullet) by a factor of 100.
- Maximum Permissible Concentration (MPC) concentration in an environmental compartment at which:
  - 1. no effect to be rated as negative is to be expected for ecosystems;
  - 2a no effect to be rated as negative is to be expected for humans (for non-carcinogenic substances);
  - 2b for humans no more than a probability of 10<sup>-6</sup> over the whole life (one additional cancer incident in 10<sup>6</sup> persons taking up the substance concerned for 70 years) can be calculated (for carcinogenic substances) (Lepper, 2005).
- Maximum Acceptable Concentration (MAC<sub>eco</sub>) concentration protecting aquatic ecosystems for effects due to short-term exposure or concentration peaks.
- Serious Risk Concentration (SRC<sub>eco</sub>) concentration at which serious negative effects in an ecosystem may occur.

It should be noted that ERLs are scientifically derived values, based on (eco)toxicological, fate and physico-chemical data. They serve as advisory values for the Dutch Steering Committee for Substances, which is appointed to set the Environmental Quality Standards (EQSs) from these ERLs. ERLs should thus be considered as preliminary values that do not have any official status.

### 1.2 Production and use of acrylonitrile

According to the Risk Assessment Report (RAR) (European Commission, 2004), acrylonitrile is produced in a closed system by catalytic ammoxidation of ammonia and propylene. Fractional distillation of the crude (85%) product following scrubbing to remove ammonia yields 99.9% pure acrylonitrile. In the RAR of 2004 is reported that the current production volume in the EU is in excess of 1,250,000 tonnes per year. Acrylonitrile is now used almost exclusively as a monomer in the production of polymeric materials, with some use as a precursor for acrylamide and adiponitrile. Acrylonitrile can therefore be regarded as an industrial intermediate. More details can be found in the RAR (European Commission, 2004).

### 2 Methods

#### 2.1 Data collection

The final Risk Assessment Report (RAR) of acrylonitrile (European Commission, 2004) produced in the framework of Existing Substances Regulation (793/93/EEC) was used as only source of physicochemical and (eco)toxicity data. Information given in the RARs is checked thoroughly by European Union member states (Technical Committee) and afterwards approved by the Scientific Commission on Health and Environmental Risk (SCHER). Therefore, no additional evaluation of data is performed for the ERL derivation. Only valid data combined in an aggregated data table are presented in the current report. Occasionally, key studies are discussed when relevant for the derivation of a certain ERL.

In the aggregated data table only one effect value per species is presented. When for a species several effect data are available, the geometric mean of multiple values for the same endpoint is calculated where possible. Subsequently, when several endpoints are available for one species, the lowest of these endpoints (per species) is reported in the aggregated data table.

### 2.2 Methodology for derivation of environmental risk limits

The methodology for data selection and ERL derivation is described in Van Vlaardingen and Verbruggen (2007) which is in accordance with Lepper (2005). For the derivation of ERLs for air, no specific guidance is available. However, as much as possible the basic principles underpinning the ERL derivation for the other compartments are followed for the atmospheric ERL derivation (if relevant for a chemical).

#### 2.2.1 Drinking water abstraction

The INS-Guidance includes the MPC for surface waters intended for the abstraction of drinking water (MPC $_{dw, water}$ ) as one of the MPCs from which the lowest value should be selected as the general MPC $_{water}$  (see INS-Guidance, Section 3.1.6 and 3.1.7). According to the proposal for the daughter directive Priority Substances, however, the derivation of the AA-EQS (= MPC) should be based on direct exposure, secondary poisoning, and human exposure due to the consumption of fish. Drinking water was not included in the proposal and is thus not guiding for the general MPC $_{water}$  value. The exact way of implementation of the MPC $_{dw, water}$  in the Netherlands is at present under discussion within the framework of the "AMvB Kwaliteitseisen en Monitoring Water". No policy decision has been taken yet, and the MPC $_{dw, water}$  is therefore presented as a separate value in this report.

The  $MPC_{dw, water}$  is also used to derive the  $MPC_{gw}$ . For the derivation of the  $MPC_{dw, water}$ , a substance specific removal efficiency related to simple water treatment may be needed. Because there is no agreement as yet on how the removal fraction should be calculated, water treatment is not taken into account.

#### 2.2.2 MAC<sub>eco, marine</sub>

In this report, a  $MAC_{eco}$  is also derived for the marine environment. The assessment factor for the  $MAC_{eco,\,marine}$  value is based on:

- the assessment factor for the MAC<sub>eco, water</sub> value, when acute toxicity data for at least two specific marine taxa are available, or
- using an additional assessment factor of 5, when acute toxicity data for only one specific marine taxon are available (analogous to the derivation of the MPC according to Van Vlaardingen and Verbruggen (2007)), or
- using an additional assessment factor of 10, when no acute toxicity data are available for specific marine taxa.

If freshwater and marine data sets are not combined the  $MAC_{eco,\,marine}$  is based on the marine toxicity data using the same additional assessment factors as mentioned above. It has to be noted that this procedure is currently not agreed upon. Therefore, the  $MAC_{eco,\,marine}$  value needs to be re-evaluated once an agreed procedure is available.

# 3 Derivation of environmental risk limits for acrylonitrile

# 3.1 Substance identification, physico-chemical properties, fate and human toxicology

### 3.1.1 Identity

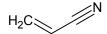


Figure 1. Structural formula of acrylonitrile.

Table 2. Identification of acrylonitrile.

Parameter	Name or number
Chemical name	2-propenenitrile
Common/trivial/other name	vinyl cyanide, cyanoethylene, acrylonitrile
CAS number	107-13-1
EC number	203-466-5
Molecular formula:	$C_3H_3N$

#### 3.1.2 Physico-chemical properties

Table 3. Physico-chemical properties of acrylonitrile, for original overview and references see De Jong et al. (2007).

Parameter	Unit	Value	Remark
Molecular weight	[g.mol <sup>-1</sup> ]	53.06	
Water solubility	$[g.L^{-1}]$	73.5	20°C
$\log K_{ m OW}$	[-]	0.25	shake-flask
$K_{\rm OC}$	$[L.kg^{-1}]$	14.1	calculated from Log Kow 0.25
Vapour pressure	[Pa]	$1.33 \times 10^5$	22.8 °C
Melting point	[°C]	-83.6	
Boiling point	[°C]	77.3	
Henry's law constant	[Pa.m <sup>3</sup> .mol <sup>-1</sup> ]	9.6	

n.a. = not applicable.

#### 3.1.3 Behaviour in the environment

Table 4. Selected environmental properties of acrylonitrile.

Parameter	Unit	Value	Remark
Hydrolysis half-life	DT50 [d]	n.a.	
Photolysis half-life	DT50 [d]	5	based on oxidation with OH
Degradability			not readily biodegradable

#### Ouote from the RAR:

"Acrylonitrile monomer released to the environment as a consequence of production or further processing will distribute primarily to the atmosphere and to the aqueous environment. Redistribution to other environmental compartments is anticipated to be negligible. There is rapid photodegradation of acrylonitrile, while in the aquatic environment acrylonitrile, while not readily biodegradable based on available information, appears to degrade rapidly in wastewater treatment plants following acclimation, and also degrades in surface water. Up to 99% biodegradation has been reported in simulation tests."

#### 3.1.4 Bioconcentration and biomagnification

An overview of the bioaccumulation data for acrylonitrile is given in Table 5.

Table 5. Overview of bioaccumulation data for acrylonitrile.

Parameter	Unit	Value	Remark	
BCF (fish)	[L.kg <sup>-1</sup> ]	48	experimental value based on <sup>14</sup> C uptake,	
			according to RAR probably too high because the	
			value is attributable to binding of acrylonitrile to	
			tissue macromolecules rather than to true	
			bioaccumulation (see RAR)	
BCF (fish)	[L.kg <sup>-1</sup> ] [kg.kg <sup>-1</sup> ]	1.41	calculated in the RAR with EUSES	
BMF	[kg.kg <sup>-1</sup> ]	1	default value since the BCF < 2000 L.kg <sup>-1</sup> .	

In the RAR no final BCF is selected. The QSARs in EUSES are not reliable to calculate BCF values for compounds with low  $K_{ow}$  values as acrylonitrile. Therefore, in this report is the experimental value of  $48 \text{ L.kg}^{-1}$  selected as worst case scenario.

#### 3.1.5 Human toxicology: classification and limit values

The following classification and labelling was reported in the RAR according to the 25<sup>th</sup> ATP of Directive 67/548/EEC:

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

Toxicological limit values for oral and inhalation exposure to acrylonitrile have been derived by RIVM/SIR. The EU-RAR concluded that based on the available evidence acrylonitrile should be regarded as a possible genotoxic carcinogen. For such compounds a non-threshold quantitative cancer risk assessment (QCRA) is applied in toxicological limit value derivation. For acrylonitrile an oral limit value was derived on the basis of the lower confidence limit (LCL) of an oral TD05-value obtained via

dose-response modelling using the increased incidences of nervous system tumours as found in an oral carcinogenicity study in rats (Biodynamics 1980). The LCL-TD05 of 1.4 mg.kg $_{bw-z}^{-1}$ .day $^{-1}$  (female rats) was recalculated to a lifetime cancer risk of 10<sup>-6</sup>, which is the risk level used within the present scope (Van Vlaardingen and Verbruggen 2007). The result was an oral limit value of 0.028 µg.kg<sub>bw</sub><sup>-1</sup>.day<sup>-1</sup>. For inhalation QCRA, the lower confidence limit of the inhalation TD05-value as derived from a rat inhalation study reported by Quast et al. (1980) was used as point of departure for extrapolation to the lifetime cancer risk of 10<sup>-6</sup>. Thus, based on an LCL-TD05 of 4.5 mg.m<sup>-3</sup>, obtained via dose-response modelling based on increased incidences of nervous system tumours in female rats, a lifetime cancer risk of 10<sup>-6</sup> at 0.09 μg.m<sup>-3</sup> was calculated.

#### Trigger values 3.2

This section reports on the trigger values for ERL<sub>water</sub> derivation (as demanded in WFD framework).

Table 6. Acr	ylonitrile: collected	properties fo	or comparison to	MPC triggers.

Parameter	Value	Unit	Method/Source
$\text{Log } K_{p,\text{susp-water}}$	0.045	[-]	$K_{\mathrm{OC}}  imes f_{\mathrm{OC,susp}}^{1}$
BCF	48	$[L.kg^{-1}]$	experimental
BMF	1	$[kg.kg^{-1}]$	
$\text{Log } K_{\text{OW}}$	0.25	[-]	
R-phrases	R23/24/25, 37/38-	[-]	
	41, 43, 45, 51-53		
A1 value	-	$[\mu g.L^{-1}]$	
DW standard	-	[µg.L <sup>-1</sup> ]	

 $<sup>1</sup> f_{OC,susp} = 0.1 \text{ kg}_{OC}.\text{kg}_{solid}^{-1}$  (European Commission (Joint Research Centre), 2003).

- acrylonitrile has a log  $K_{p, \text{ susp-water}} < 3$ ; derivation of MPC<sub>sediment</sub> is not triggered.
- acrylonitrile has a log  $K_{p, \text{ susp-water}} < 3$ ; expression of the MPC<sub>water</sub> as MPC<sub>susp, water</sub> is not required. acrylonitrile has a BCF < 100 L.kg<sup>-1</sup>; assessment of secondary poisoning is not triggered.
- 0
- acrylonitrile has an R23/24/25, 37/38-41, 43, 45 classification. Therefore, an MPC<sub>water</sub> for human health via food (fish) consumption (MPC<sub>hh food, water</sub>) should be derived.

#### Toxicity data and derivation of ERLs for water 3.3

Acrylonitrile has been assessed before by De Jong et al. (2007). Only those ERLs that were not derived in that report are derived here. An overview of the selected freshwater toxicity data for acrylonitrile as reported in the RAR and De Jong et al. (2007) is given in Table 7. Marine toxicity data are shown in Table 8.

Table 7. Acrylonitrile: selected freshwater toxicity data for ERL derivation.

Chronic		Acute	
Taxonomic group	NOEC/EC <sub>10</sub> (mg.L <sup>-1</sup> )	Taxonomic group	L(E)C <sub>50</sub> (mg.L <sup>-1</sup> )
Crustacea		Algae	
Daphnia magna	0.78	Scenedesmus subspicatus	3.1
Pisces		Mollusca	
Lepomis macrochirus	10.0	Radix pliculata	17.94 <sup>e</sup>
Pimephales promelas	<b>0.17</b> <sup>f</sup>	Annelida	
		Limnodrilus hoffmeisteri	16.9
		Crustacea	
		Daphnia magna	11.3 <sup>a</sup>
		Insecta	
		Chironomus sp.	14.21
		Pisces	
		Danio rerio	15.0
		Carrasius sp.	40.0
		Cyprinus carpio	21.7 <sup>b</sup>
		Lebistes reticulatus	33.5
		Lepomis macrochirus	10.9 <sup>c</sup>
		Leucaspius delineatus	22.7
		Leuciscus idus	21.2
		Oncorhynchus mykiss	13.0 <sup>d</sup>
		Phoxinus phoxinus	17.6
		Pimephales promelas	10.1 <sup>e</sup>
		Rhodeus sericeus	25.7

Notes:

a: geometric mean of 8.7, 7.6 and 22

b: geometric mean of 19.64 and 24

c: geometric mean of 10 and 11.8

d: geometric mean of 7 and 24

e: lowest value for this species

f: is LOEC/2

Table 8. Acrylonitrile: selected marine toxicity data for ERL derivation.

Chronic		Acute	
Taxonomic group $NOEC/EC_{10}$ (mg. $\Gamma^{1}$ )		Taxonomic group	L(E)C <sub>50</sub> (mg.l <sup>-1</sup> )
Algae		Bacteria	
Skeletonema costatum	0.41 <sup>b</sup>	Vibrio fischeri	254
Pisces		Algae	
Cyprinodon variegatus	5.6	Skeletonema costatum	1.63
		Annelida	
		Ophryotrocha diadema	18.2
		Crustacea	
		Artemia salina	14.34
		Crangon crangon	10.4 <sup>a</sup>
		Pisces	
		Cyprinodon variegatus	8.6
		Gobius minutes	14.0
		Lagadon rhomboides	24.5

Notes:

a: geometric mean of 18.2 and 6  $\mu$ g.L<sup>-1</sup>.

b: lowest value, parameter biomass.

#### 3.3.1 Treatment of fresh- and saltwater toxicity data

Marine data do not indicate a difference in sensitivity between freshwater and marine species. Therefore data for freshwater and marine species are pooled.

#### 3.3.2 Mesocosm studies

No mesocosm studies are presented in the RAR.

#### 3.3.3 Derivation of MPC<sub>water</sub> and MPC<sub>marine</sub>

#### 3.3.3.1 MPC<sub>eco, water</sub> and MPC<sub>eco, marine</sub>

De Jong et al. (2007) derived an MPC<sub>eco, water</sub> of 17 μg.L<sup>-1</sup> and an MPC<sub>eco, marine</sub> of 1.7 μg.L<sup>-1</sup>. The lower value of 0.08 mg.L<sup>-1</sup> for *Radix peregra* was not used in the derivation because this value was not considered valid in the RAR and only given as supporting information.

#### 3.3.3.2 MPC<sub>sp, water</sub> and MPC<sub>sp, marine</sub>

Acrylonitrile has a BCF < 100 L.kg<sup>-1</sup>, thus assessment of secondary poisoning is not triggered.

#### 3.3.3.3 MPC<sub>hh food, water</sub>

Derivation of MPC<sub>hh food, water</sub> for acrylonitrile is triggered (Table 6). This derivation is based on the oral limit value of  $0.028~\mu g.kg_{bw}^{-1}.day^{-1}$ . MPC<sub>hh, food</sub> =  $0.1*0.028*70/0.115 = 1.7~\mu g.kg_{feed}^{-1}$ . The resulting MPC<sub>hh food, water</sub> is then:  $1.7/(48*1) = 0.036~\mu g.L^{-1}$ .

#### 3.3.3.4 Selection of the MPC<sub>water</sub> and MPC<sub>marine</sub>

The lowest value is the MPC<sub>hh food,water</sub> of  $0.036~\mu g.L^{-1}$ . This sets the final MPC<sub>water</sub> to the MPC of human health:  $0.036~\mu g.L^{-1}$ . Similarly is the final MPC<sub>marine</sub>:  $0.036~\mu g.L^{-1}$ .

#### 3.3.4 MPC<sub>dw, water</sub>

No A1 value and DW standard are available for acrylonitrile. With the oral limit value of 0.028  $\mu g.k g_{bw}^{-1}.d^{-1}$  an MPC<sub>dw, water, provisional</sub> can be calculated with the following formula: MPC<sub>dw, water, provisional</sub> = 0.1.TL<sub>hh</sub>.BW / Uptake<sub>dw</sub> where TL<sub>hh</sub> is the oral limit value, BW is a body weight of 70 kg, and uptake<sub>dw</sub> is a daily uptake of 2 L. As described in section 2.2 water treatment is currently not taken into account. Therefore the MPC<sub>dw, water</sub> = The MPC<sub>dw,water, provisional</sub> and becomes: 0.1 \* 0.028 \* 70 / 2 = 0.098  $\mu g.L^{-1}$ .

#### 3.3.5 Derivation of MAC<sub>eco</sub>

The MAC<sub>eco</sub> is based on the lowest L(E)C50. This is the algae *Skeletonema costatum* with an L(E)C50 of 1.63 mg.L<sup>-1</sup> (see Table 8). An assessment factor of 100 is applied since acryloniltrile has no potential to bioaccumulate. This sets the MAC<sub>eco, water</sub> initially to 16.3  $\mu$ g.L<sup>-1</sup>. This value is not deemed realistic since this would imply that one expects acute toxic effects at concentrations below the ERL that protects from chronic exposure (van Vlaardingen and Verbruggen 2007). Therefore is the MAC<sub>eco, water</sub> set equal to the MPC<sub>eco, water</sub>: 17  $\mu$ g.L<sup>-1</sup>.

The MAC<sub>eco, marine</sub> is set a factor 10 lower than the initial MAC<sub>eco, water</sub> since there are no data for additional marine taxa. The fish, *Cypridon variegates*, and annelinda, *Ophryotrocha diadema*, in Table 8 do not account as additional marine taxonomic groups since they have the same life form and feeding strategy as freshwater species. Therefore is the MAC<sub>eco, marine</sub> is initiall set to 1.63  $\mu$ g.L<sup>-1</sup>. This value is lower than the MPC<sub>eco, marine</sub> of 1.7  $\mu$ g.L<sup>-1</sup>. Therefore is the MAC<sub>eco, marine</sub> set equal to the

MPC<sub>eco, marine</sub>:  $1.7 \mu g.L^{-1}$ .It has to be noted that this procedure for the MAC<sub>eco, marine</sub> is currently not agreed upon. Therefore, the MAC<sub>eco, marine</sub> needs to be re-evaluated once an agreed procedure is available.

#### 3.3.6 Derivation of NC

Negligible concentrations are derived by dividing the MPCs by a factor 100. This gives an  $NC_{water}$  of 0.36 ng.L<sup>-1</sup> and an  $NC_{marine}$  of 0.36 ng.L<sup>-1</sup>

#### 3.3.7 Derivation of SRC<sub>eco, aquatic</sub>

De Jong et al. (2007) derived an SRC<sub>eco, aquatic</sub> of 1.25 mg.L<sup>-1</sup>. The SRC<sub>eco, aquatic</sub> is valid for the marine and the freshwater environment.

#### 3.4 Toxicity data and derivation of ERLs for sediment

The  $\log K_{\rm p, \, susp-water}$  of acrylonitrile is below the trigger value of 3, therefore, ERLs are not derived for sediment.

#### 3.5 Toxicity data and derivation of ERLs for soil

No data for soil organisms has been presented in the EU-RAR.

#### 3.5.1 Derivation of the MPC<sub>soil</sub>

#### 3.5.1.1 MPC<sub>eco, soil</sub>

De Jong et al. (2007) derived an MPC<sub>soil</sub> of 0.021 mg.kg<sub>dwt</sub><sup>-1</sup> for Dutch standard soil.

#### 3.5.1.2 MPC<sub>human, soil</sub>

For the derivation of the MPC  $_{human, \, soil}$ , the oral limit value of 0.028  $\mu g.k g_{bw}^{-1}.day^{-1}$  can be used as  $TL_{hh}$  with the method as described in Van Vlaardingen and Verbruggen (2007). For this calculation, the log  $K_{ow}$ , log  $K_{oc}$  and Henry coefficient are the same as used by De Jong et al. (2007). For the solubility, the value from table 3 has been used. This is the geometric mean of all solubility data presented in De Jong et al. (2007). Specific human intake routes are allowed to contribute 10% of the human toxicological threshold limit. Four different routes contributing to human exposure have been incorporated: consumption of leafy crops, root crops, milk and meat. Uptake via root crops was determined to be the critical route. The calculated MPC  $_{human, \, soil}$  is 0.66  $\mu g.k g_{dwt}^{-1}$  for Dutch standard soil.

#### 3.5.1.3 Selection of the MPC<sub>soil</sub>

Since the MPC<sub>human soil</sub> is the lowest value, the MPC<sub>soil</sub> is 0.66 µg,kg<sub>dwt</sub><sup>-1</sup> for Dutch standard soil.

#### 3.5.2 Derivation of NC<sub>soil</sub>

Negligible concentrations are derived by dividing the MPCs by a factor 100. This gives an  $NC_{soil}$  of 6.6 ng. $kg_{dw}^{-1}$ .

#### 3.5.3 Derivation of SRC<sub>eco, soil</sub>

De Jong et al. (2007) derived an SRC<sub>eco. soil</sub> of 1.5 mg.kg<sub>dwt</sub><sup>-1</sup> for Dutch standard soil.

### 3.6 Derivation of ERLs for groundwater

#### 3.6.1 Derivation of MPC<sub>gw</sub>

#### 3.6.1.1 MPC<sub>eco, gw</sub>

Since groundwater-specific exotoxicological information for the groundwater compartment is absent, the surface water MPC<sub>eco, water</sub> is taken as substitute. De Jong et al. (2007) derived an MPC<sub>eco, water</sub> of  $17 \mu g.L^{-1}$  Thus, MPC<sub>eco, gw</sub> = MPC <sub>eco, water</sub> =  $17 \mu g.L^{-1}$ .

#### 3.6.1.2 MPC<sub>human, gw</sub>

The MPC<sub>human, gw</sub> is set equal to the MPC<sub>dw, water</sub>. Therefore the MPC<sub>human, gw</sub> = MPC<sub>dw, water</sub>:  $0.098 \ \mu g.L^{-1}$ .

#### 3.6.1.3 Selection of $MPC_{gw}$

The lowest MPC<sub>gw</sub> is the MPC<sub>human, gw</sub> which makes the MPC<sub>gw</sub>: 0.098 μg.L<sup>-1</sup>.

#### 3.6.2 Derivation of NC<sub>gw</sub>

Negligible concentrations are derived by dividing the MPCs by a factor 100. This gives an  $NC_{gw}$  of 0.98 ng.L<sup>-1</sup>.

#### 3.6.3 Derivation of SRC<sub>eco, gw</sub>

The SRC<sub>eco, gw</sub> is set equal to the SRC<sub>eco, water</sub>. Therefore the SRC<sub>eco, gw</sub> is: 1.25 mg.L<sup>-1</sup>.

#### 3.7 Derivation of ERLs for air

#### 3.7.1 Derivation of the MPC<sub>air</sub>

#### 3.7.1.1 MPC<sub>eco, air</sub>

In the RAR a PNEC<sub>air</sub> has been derived using LC50 data for a number of insect species and assuming a conservative figure of 0.5 mg.L<sub>air</sub><sup>-1</sup> for the LC50 gives. The derived PNEC is 0.5  $\mu$ g.L<sub>air</sub><sup>-1</sup>. This value can be taken over as an MPC<sub>eco, air</sub> of 0.5 mg.m<sup>-3</sup>.

#### 3.7.1.2 Derivation of MPC<sub>human, air</sub>

In section 3.1.5 an inhalation limit value of 0.09  $\mu g.m^{-3}$  has been derived. This value will be set as the MPC<sub>human, air</sub>. The MPC<sub>human, air</sub> is: 0.09  $\mu g.m^{-3}$ .

#### 3.7.1.3 Selection of the MPC<sub>air</sub>

The lowest MPC<sub>air</sub> available is the MPC<sub>human, air</sub> so the MPC for air will be the MPC<sub>human, air</sub>: 90 ng.m<sup>-3</sup>.

#### 3.7.2 Derivation of NC<sub>air</sub>

The MPC<sub>air</sub> divided by 100 is the NC<sub>air</sub>: 0.90 ng.m<sup>-3</sup>

### 3.8 Comparison of derived ERLs with monitoring data

The RIWA (Dutch Association of River Water companies, www.riwa.org) does not present any surface water monitoring for acrylonitrile in their annual reports between 2001 and 2006. Also the Dutch Ministry of Transport, Public Works and Water Management does not present any monitoring data for acrylonitrile on their website (<a href="www.waterstat.nl">www.waterstat.nl</a>). Therefore, no comparison of the derived ERLs with monitoring data is possible.

### 4 Conclusions

In this report, the risk limits Negligible Concentration (NC), Maximum Permissible Concentration (MPC), Maximum Acceptable Concentration for ecosystems (MAC $_{\rm eco}$ ), and Serious Risk Concentration for ecosystems (SRC $_{\rm eco}$ ) are derived for acrylonitrile in water, groundwater, soil and air. The ERLs that were obtained are summarised in the table below. Monitoring data for acrylonitrile in the Dutch environment are not available. Therefore it cannot be judged if the derived ERLs are being exceeded.

Table 9. Derived MPC, NC, MAC<sub>eco</sub>, and SRC values for acrylonitrile.

ERL	unit	value			
		MPC	NC	$MAC_{eco}$	$SRC_{eco}$
water <sup>a</sup>	ng.L <sup>-1</sup>	36	0.36	$1.7 \times 10^4$	$1.3 \times 10^6$
drinking water b	ng.L <sup>-1</sup>	98			
marine	ng.L <sup>-1</sup>	36	0.36	$1.7 \times 10^3$	$1.3 \times 10^6$
sediment	μg.kg <sub>dwt</sub> -1	n.d.			
soil <sup>c</sup>	μg.kg <sub>dwt</sub> -1	0.66	$6.6 \times 10^{-3}$		$1.5 \times 10^3$
groundwater	μg.kg <sub>dwt</sub> -1 μg.kg <sub>dwt</sub> -1 ng.L <sup>-1</sup>	98	0.98		$1.3 \times 10^6$
air	ng.m <sup>-3</sup>	90	0.90		

<sup>&</sup>lt;sup>a</sup> From the MPC<sub>eco, water</sub>, MPC<sub>sp, water</sub> and MPC<sub>hh, food, water</sub> the lowest one is selected as the 'overall' MPC<sub>water</sub>.

<sup>&</sup>lt;sup>b</sup> The exact way of implementation of the  $MPC_{dw, water}$  in the Netherlands is at present under discussion. Therefore, the  $MPC_{dw, water}$  is presented as a separate value in this report.

<sup>&</sup>lt;sup>c</sup> Expressed on the basis of Dutch standard soil.

n.d. = not derived.

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