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## Environmental risk limits for toluene

RIVM letter report 601782005/2008

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

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## **Rapport in het kort**

### **Environmental risk limits for toluene**

Dit rapport geeft milieurisicogrenzen voor toluen in (grond)water, lucht en bodem. Milieurisicogrenzen zijn de technisch-wetenschappelijke advieswaarden voor de uiteindelijke milieukwaliteitsnormen in Nederland. De milieurisicogrenzen voor toluen zijn gebaseerd op de uitkomsten van de EU risicobeoordeling voor toluen (Bestaande Stoffen Verordening 793/93). De afleiding van de milieurisicogrenzen sluit tevens aan bij de richtlijnen uit de Kaderrichtlijn Water.



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## Summary

Environmental risk limits (ERLs) are derived using ecotoxicological, physicochemical, 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 toluene 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 based on data presented in the Risk Assessment Report (RAR), created under the European Existing Substances Regulation (793/93/EEC). No risk limits were derived for the sediment compartment, because exposure of sediment is considered negligible.

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  $SRC_{eco}$  and for the ERLs for the soil and atmospheric compartment, 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.

**Table 1. Derived MPC, NC,  $MAC_{eco}$ , and  $SRC_{eco}$  values for toluene.**

ERL	Unit	MPC	NC	$MAC_{eco}$	$SRC_{eco}$
Water <sup>a</sup>	$\mu\text{g.l}^{-1}$	74	0.74	550	5,700
Drinking water <sup>a</sup>	$\mu\text{g.l}^{-1}$	1,700			
Marine	$\mu\text{g.l}^{-1}$	7.4	0.07	55 <sup>c</sup>	5,700
Sediment		n.d. <sup>b</sup>			
Soil <sup>d</sup>	$\mu\text{g.kg}_{dw}^{-1}$	880	8.8		$4.0 \times 10^5$
Groundwater	$\mu\text{g.l}^{-1}$	74	0.74		
Air	$\mu\text{g.m}^{-3}$	400	4.0		

<sup>a</sup> The  $MPC_{dw, water}$  is reported as a separate value from the other  $MPC_{water}$  values ( $MPC_{eco, water}$ ,  $MPC_{sp, water}$  or  $MPC_{hh, food, water}$ ). From these other  $MPC_{water}$  values (thus excluding the  $MPC_{dw, water}$ ) the lowest one is selected as the 'overall'  $MPC_{water}$ .

<sup>b</sup> n.d. = not determined.

<sup>c</sup> provisional value.

<sup>d</sup> expressed on Dutch standard soil

# 1 Introduction

## 1.1 Project framework

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

- 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  $10^{-6}$  over the whole life (one additional cancer incident in  $10^6$  persons taking up the substance concerned for 70 years) can be calculated (for carcinogenic substances) (Lepper, 2005).
- maximum acceptable concentration ( $MAC_{eco}$ ) – concentration protecting aquatic ecosystems for effects due to short-term exposure or concentration peaks.
- serious risk concentration ( $SRC_{eco}$ ) – concentration at which serious negative effects in an ecosystem may occur.

It should be noted that ERLs are scientifically (based on (eco)toxicological, fate and physico-chemical data) 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.

## 2 Methods

### 2.1 Data collection

The final Risk Assessment Report (RAR) of toluene agreed upon within the framework of the Existing Substances Regulation (793/93/EEC) was used as only source of physico-chemical and (eco)toxicity data (Environmental Chemicals Bureau, 2003) Information given in the RAR is checked thoroughly by European Union Member States (Technical Committee) and 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 present 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.

For the derivation of risk limits for human health, an expert from the RIVM is consulted to appoint the most recent and relevant Tolerable Daily Intake (TDI) and/or Tolerable Concentration in Air (TCA), if available.

### 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) that 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).

## 3 Derivation of environmental risk limits

### 3.1 Toluene

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

##### 3.1.1.1 Identity

Figure 1. Structural formula of toluene.

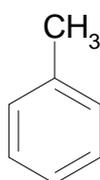


Table 2. Identification of toluene.

Parameter	Name or number
Chemical name	Toluene
Common/trivial/other name	Methylbenzene, phenyl methane, toluol, methyl benzol, methacide
CAS number	108-88-3
EC number	203-625-9
SMILES code	c1ccccc1C

##### 3.1.1.2 Physico-chemical properties

Table 3. Physico-chemical properties of toluene, derived from the RAR. The values presented below were used for risk assessment under the Existing Substances Regulation (793/93/EEC).

Parameter	Unit	Value	Remark
Molecular weight	[g.mol <sup>-1</sup> ]	92.5	
Water solubility	[mg.l <sup>-1</sup> ]	515	At 20°C
Water solubility	[mg.l <sup>-1</sup> ]	534.8	At 25°C
log <i>K</i> <sub>OW</sub>	[-]	2.65	measured
log <i>K</i> <sub>OC</sub>	[-]	2.25	<i>K</i> <sub>OC</sub> = 177
Vapour pressure	[Pa]	3000	At 20°C
Vapour pressure	[Pa]	3800	At 25°C
Melting point	[°C]	-95	

Boiling point	[°C]	110.6	At 1013 hPa
Henry's law constant	[Pa.m <sup>3</sup> .mol <sup>-1</sup> ]	537	At 20°C

### 3.1.1.3 Behaviour in the environment

Table 4. Selected environmental properties of toluene, derived from the RAR.

Parameter	Unit	Value	Remark
Hydrolysis half-life	DT <sub>50</sub> [d]	-	No experimental data, but hydrolysis is not expected to occur under normal environmental conditions
Photolysis half-life	DT <sub>50</sub> [d]	2	See paragraph below
Degradability		Ready biodegradable	See paragraph below
Relevant metabolites		n.r. <sup>a</sup>	

<sup>a</sup> not reported for the environment

The direct photolytic degradation of toluene is estimated to be negligible in the RAR. Indirect photolysis by photochemical oxidative degradation was observed in air. The most important atmospheric removal process for toluene is by reaction with the OH radical.

Toluene is ready biodegradable in several standard biodegradability tests using sewage sludge inoculums. The degradation rate in surface waters was estimated to correspond with a DT<sub>50</sub>-value of 30 days. This result was used in the estimations of the regional environmental concentrations of toluene in the RAR.

### 3.1.1.4 Bioconcentration and biomagnification

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

Table 5. Overview of bioaccumulation data for toluene, reported in the RAR for toluene.

Parameter	Unit	Value	Remark
BCF (fish)	[l.kg <sup>-1</sup> ]	90 <sup>1</sup>	Chosen as worst case scenario in risk assessment
BCF (mussel)	[l.kg <sup>-1</sup> ]	4.2 <sup>2</sup>	
BMF	[kg.kg <sup>-1</sup> ]	n.a. <sup>3</sup>	

<sup>1</sup> for *Leuciscus idus melanotus*, highest value for fish from three studies

<sup>2</sup> for *Mytilus edulis*

<sup>3</sup> n.a. = not available

In the RAR it was concluded that the low bioaccumulation potential in fish and molluscs and the rapid elimination rate indicate that toluene is unlikely to bioconcentrate in the aquatic food chain.

### 3.1.1.5 Human toxicological threshold limits and carcinogenicity

In the RAR and Annex I of 67/548/EEC, toluene was classified as follows:

F, R11	Highly flammable.
Repr.Cat.3; R63	Possible risk of harm to the unborn child.
Xn; R48/20-65	Harmful: danger of serious damage to health by prolonged exposure through inhalation. May cause lung damage if swallowed.
Xi; R38	Irritating to skin.
R67	Vapors may cause drowsiness and dizziness.

In the RAR for toluene, an oral NOAEL of  $625 \text{ mg.kg bw}^{-1}.\text{day}^{-1}$  is used. This NOAEL is based on a 90-day rat study with oral dosing. The WHO (WHO, 1991-1996) considered this NOAEL to be a LOAEL and calculated a TDI of  $223 \text{ }\mu\text{g.kg}_{\text{bw}}^{-1}.\text{day}^{-1}$  as oral limit on basis of this value. The TDI is appointed as starting point for the current ERL-derivation.

### 3.1.2 Trigger values

This section reports on the trigger values for  $\text{ERL}_{\text{water}}$  derivation (as demanded in WFD framework).

Table 6. Toluene: collected properties for comparison to MPC triggers for the water compartment.

Parameter	Value	Unit	Method/Source	Derived at section
$\log K_{\text{P, susp-water}}$	1.25	[-]	$K_{\text{OC}} \times f_{\text{OC, susp}}^1$	$K_{\text{OC}}$ : 3.1.1.2
BCF	90	$[\text{l.kg}^{-1}]$		3.1.1.4
BMF	n.r.	[-]		3.1.1.4
$\log K_{\text{OW}}$	2.65	[-]		3.1.1.2
R-phrases	R63, R48/20-65, R38, R67	[-]		3.1.1.5
A1 value	n.a. <sup>2</sup>	$[\mu\text{g.l}^{-1}]$		
DW standard	n.a. <sup>2</sup>	$[\mu\text{g.l}^{-1}]$		

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

<sup>2</sup>n.a. = not available

- Toluene has a  $\log K_{\text{P, spm-water}} < 3$ ; derivation of  $\text{MPC}_{\text{sediment}}$  is not triggered.
- Toluene has a  $\log K_{\text{P, spm-water}} < 3$ ; expression of the  $\text{MPC}_{\text{water}}$  as  $\text{MPC}_{\text{susp, water}}$  is not required.
- Toluene has a  $\text{BCF} < 100$ ; assessment of secondary poisoning is not triggered.
- Toluene has an R63, R48/20-65, R38, R67 classification. Therefore, an  $\text{MPC}_{\text{water}}$  for human health via food (fish) consumption ( $\text{MPC}_{\text{hh food, water}}$ ) needs to be derived.
- For toluene, no A1 and no Drinking Water value are available from Council Directives 75/440/EEC and 98/83/EC, respectively. Therefore, a provisional DWS needs to be derived.

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

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

An overview of the selected freshwater toxicity data for toluene is given in Table 7. Marine toxicity data are shown in Table 8.

Table 7. Toluene: selected aquatic freshwater data for ERL derivation.

Chronic <sup>a</sup>		Acute <sup>a</sup>	
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> )
<b>Bacteria</b>		<b>Bacteria</b>	
<i>Pseudomonas putida</i>	29	<i>Nitrosomonas</i>	84
		<i>Pseudomonas putida</i>	193
<b>Protozoa</b>		<b>Protozoa</b>	
<i>Entosiphon sulcatum</i>	456	<i>Tetrahymena pyriformis</i>	289
<b>Algae</b>		<b>Algae</b>	
<i>Scenedesmus quadricauda</i>	> 400	<i>Chlamydomonas angulosa</i>	134
<i>Selenastrum carpicornutum</i>	10	<i>Chlorella vulgaris</i>	207
<i>Skeletonema costatum</i>	10	<i>Scenedesmus quadricauda</i>	> 433
<b>Crustacea</b>		<b>Crustacea</b>	
<i>Ceriodaphnia dubia</i>	0.74	<i>Ceriodaphnia dubia</i>	3.78
<i>Daphnia magna</i>	0.87 <sup>b</sup>	<i>Daphnia magna</i>	13.1
<b>Pisces</b>		<b>Pisces</b>	
<i>Oncorhynchus kisutch</i>	1.4	<i>Carassius auratus</i>	22.8
<i>Oncorhynchus mykiss</i>	2.6 <sup>c</sup>	<i>Lepomis macrochirus</i>	13
<i>Pimephales promelas</i>	4	<i>Oncorhynchus kisutch</i>	5.5
		<i>Pimephales promelas</i>	28.7 <sup>d</sup>

<sup>b</sup> Geomean of 0.53 and 1.0 mg.l<sup>-1</sup>. The value of 1.0 mg.l<sup>-1</sup> is used for SRC<sub>eco</sub> derivation.

<sup>c</sup> Geomean of 1.4 and 4.7 mg.l<sup>-1</sup>.

<sup>d</sup> Geomean of 26 and 31.7 mg.l<sup>-1</sup>.

Table 8. Toluene: selected marine data for ERL derivation.

Chronic <sup>a</sup>		Acute <sup>a</sup>	
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> )
<b>Algae</b>		<b>Algae</b>	
<i>Chlorella</i> sp.	< 34	<i>Chlorella</i> sp.	> 342
		<b>Crustacea</b>	
		<i>Artemia salina</i>	33
		<i>Cancer magister</i>	28
		<i>Chaetogammarus marinus</i>	18
		<i>Crangon franciscorum</i>	3.5
		<i>Nitocra spinipes</i>	42.4 <sup>b</sup>
		<i>Palaemonetes pugio</i>	22.9 <sup>c</sup>
<b>Pisces</b>		<b>Pisces</b>	
<i>Cyprinodon variegatus</i>	3.2	<i>Cyprinodon variegatus</i>	13
		<i>Morone saxatilis</i>	6.3

<i>Oncorhynchus gorbuscha</i>	6.1 <sup>d</sup>
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<sup>b</sup> Geomean of two separate values for a 24 h study at different salinities, i.e. 24.2 and 74.2 mg.l<sup>-1</sup>

<sup>c</sup> Geomean of four values from two separate studies performed at two different salinities. Original LC<sub>50</sub>-values were 30.6, 25.8, 20.2 and 17.2 mg.l<sup>-1</sup>.

<sup>d</sup> Geomean of 5.4 and 7 mg.l<sup>-1</sup>.

### Treatment of fresh- and saltwater toxicity data

Marine species were listed in the same table as the freshwater species in the RAR for toluene. No separate PNEC for the marine environment was derived in the RAR.

On basis of the acute and chronic data presented above, toxicity to marine and freshwater species is estimated to be similar. Therefore, the ERLs for marine or freshwater species are both based on the combined data for marine and freshwater species.

### Derivation of MPC<sub>eco, water</sub> and MPC<sub>eco, marine</sub>

The MPC<sub>eco, water</sub> is set equal to the PNEC<sub>aquatic organisms</sub> derived in the RAR.

In the RAR for toluene, the lowest long-term NOEC of 0.74 mg.l<sup>-1</sup> on *Ceriodaphnia* reproduction is chosen to base the PNEC<sub>aquatic organisms</sub> on. The base set of acute EC<sub>50</sub> from fish, daphnids and algae was concluded to be complete. Moreover, long-term NOECs from fish, *Daphnia* and algae are available. The assessment factor applied is 10 according to the TGD -> PNEC<sub>aquatic organisms</sub> = 0.74/10 = 0.074 mg.l<sup>-1</sup> = 74 µg.l<sup>-1</sup>. It is not explicitly mentioned in the RAR if this PNEC applies to both the freshwater and the marine environment.

The MPC<sub>eco, water</sub> is equal to the PNEC<sub>aquatic organisms</sub> of 0.074 mg.l<sup>-1</sup> = 74 µg.l<sup>-1</sup>. When following the TGD and using the same dataset an assessment factor of 100 should be applied to the lowest long-term NOEC of 0.74 mg.l<sup>-1</sup> -> MPC<sub>eco, marine</sub> = 7.4 µg.l<sup>-1</sup>.

In the RAR, an individual PNEC<sub>microorganisms</sub> is derived<sup>1</sup>. In the framework of ERL, microorganisms are used for the derivation of MPC<sub>eco, water</sub> and MPC<sub>eco, marine</sub>. No separate MPC<sub>microorganisms</sub> is applicable. However, since tests with microorganisms did not result in lower toxicity data compared to toxicity data for the other freshwater and marine organisms, the MPC<sub>eco, water</sub> and MPC<sub>eco, marine</sub> do not have to be adapted for microorganism sensitivity.

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

Toluene has a BCF<100, thus the assessment of secondary poisoning is not triggered.

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

The MPC<sub>hh food, water</sub> is based on the TDI of 223 µg.kg<sub>bw</sub><sup>-1</sup>. MPC<sub>hh, food</sub> = 0.1 \* 223 \* 70/0.115 = 13.6 mg.kg<sub>feed</sub><sup>-1</sup>. The resulting MPC<sub>hh food, water</sub> is 13.6/30 = 452 µg.l<sup>-1</sup>.

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

No A1 value and DW standard are available. The TL<sub>hh</sub> = TDI of 223 µg.kg<sub>bw</sub><sup>-1</sup>. The MPC<sub>dw, water, provisional</sub> = 0.1\*223\*70/2 = 780 µg.l<sup>-1</sup>. According to Zwolsman et al. (2004) the fraction not removable by simple surface water treatment amounts to 0.45 for toluene (evaporation is the main removal step). The MPC<sub>dw, water</sub>, then becomes 780/0.45= 1730 µg.l<sup>-1</sup>.

<sup>1</sup> In the RAR for toluene, for the derivation of the PNEC<sub>microorganisms</sub>, the inhibition of microbial nitrification was preferred over inhibition of respiration. The PNEC<sub>microorganisms</sub> of 84/10 = 8.4 mg.l<sup>-1</sup> was used for risk characterization.

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

In the Fraunhofer document (Lepper, 2005) it is prescribed that the lowest MPC value should be selected as the general MPC. In the proposal for the daughter directive Priority Substances, a standard based on drinking water was not included. In the Netherlands no policy decision has been taken yet on the procedure to be followed for drinking water. Therefore, in this report the MPC<sub>dw, water</sub> is reported separately (1730 µg.l<sup>-1</sup>). The lowest MPC<sub>water</sub> is 74 µg.l<sup>-1</sup> (MPC<sub>eco, water</sub>). However, the lowest reported odour threshold in water is 24 µg.l<sup>-1</sup>.

The MPC<sub>eco, arine</sub> = 7.4 µg.l<sup>-1</sup>.

### 3.1.3.6 MAC<sub>eco, water</sub> and MAC<sub>eco, marine</sub>

In the RAR for toluene, the LC<sub>50</sub>-value for *Oncorhynchus kisutch* is appointed as lowest most reliable acute value (5.5 mg.l<sup>-1</sup>), used for risk assessment. Since toluene has no potential to bioaccumulate, but acute toxicity data for different species differ more than a factor 3, an assessment factor of 10 is applied. The MAC<sub>eco</sub> for freshwater is 5.5/10 = 550 µg.l<sup>-1</sup> and for marine systems 5.5/100 = 55 µg.l<sup>-1</sup>. It has to be noted that this procedure for MAC<sub>eco, marine</sub> is currently not agreed upon. Therefore, the MAC<sub>eco, marine</sub> value needs to be re-evaluated once an agreed procedure is available.

### 3.1.3.7 NC<sub>water</sub>

The NC<sub>water</sub> is set to a factor of 100 below the final, integrated MPC<sub>water</sub>. Thus, the NC<sub>water</sub> is 0.74 µg.l<sup>-1</sup>. The NC<sub>marine</sub> = 7.4/100 = 0.074 µg.l<sup>-1</sup>.

### 3.1.3.8 SRC<sub>eco, water</sub>

#### Freshwater

Since NOECs are available for more than three taxa, the SRC<sub>eco, freshwater</sub> for the aquatic compartment is calculated as the geometric mean of the chronic toxicity data. The SRC<sub>eco, freshwater</sub> = 5.7 mg.l<sup>-1</sup>.

#### Marine

The SRC<sub>eco</sub> for the marine aquatic compartment, SRC<sub>eco, marine</sub>, is set equal to the SRC<sub>eco, water</sub>. SRC<sub>eco, marine</sub> = 5.7 mg.l<sup>-1</sup>.

## 3.1.4 Toxicity data and derivation of ERLs for sediment

No studies on sediment dwelling organisms were available in the RAR for toluene. Because the log K<sub>OW</sub> of toluene is < 3, no PNEC<sub>sediment</sub>, MPC<sub>sediment</sub> and NC<sub>sediment</sub> were calculated.

## 3.1.5 Toxicity data and derivation of ERLs for soil

Acute and chronic toxicity tests with terrestrial plants, earthworms, microbial processes and microbial cultures are summarised in the RAR for toluene. An overview of the selected soil toxicity data for toluene is given in Table 9.

Table 9. Toluene: selected soil data for ERL derivation.

Chronic		Acute	
Taxonomic group	NOEC/EC <sub>10</sub> [mg.kg dw <sup>-1</sup> ]	Taxonomic group	L(E)C <sub>50</sub> [mg.kg dw <sup>-1</sup> ]
<b>Microbial processes</b>		<b>Microbial processes</b>	
Ammonification	332 <sup>f</sup>	Respiration <sup>d</sup>	310-430
Respiration	684 <sup>g</sup>		
Nitrification	13 <sup>e</sup>		
<b>Annelida</b>			

<i>Eisenia foetida</i>	75 <sup>c</sup> 140 <sup>c</sup> 15 <sup>b</sup>
<b>Macrophyta</b>	
Maize	100 <sup>c</sup>
Fescue	1,000 <sup>c</sup>
Soybean	400 <sup>c</sup>

<sup>b</sup> Used for risk assessment. Based on visual inspection of earthworm condition

<sup>c</sup> Based on LOECs divided by two. At LOEC level, 10% yield reduction was observed.

<sup>d</sup> Respiration was tested with mix of twelve strains of aerobic microbial cultures. Test duration ten hours.

<sup>e</sup> LOEC divided by two.

<sup>f</sup> Geomean of 100 and 1,100 mg.kg<sub>dw</sub><sup>-1</sup>.

<sup>g</sup> Geomean of 360 and 1,300 mg.kg<sub>dw</sub><sup>-1</sup>.

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

The PNEC<sub>soil</sub> derivation in the RAR is reported as follows:

*'In a single 28-day study on Lactuca sativa, a yield decrease was observed at 1,000 mg.kg soil<sup>-1</sup>. In a 28-day study on earthworms, mortality, cocoon production and visual conditions were affected and the NOEC ranged between 15 and 50 mg.kg<sup>-1</sup>. In 28-day studies on soil microorganisms, the process of nitrification was the most affected process with a NOEC < 26 mg.kg soil<sup>-1</sup>. For earthworm, the NOEC (28-day) for mortality and cocoon production was ≤ 150 and < 280 mg.kg<sup>-1</sup>, respectively. However, based on visual inspection on the earthworm condition, the NOEC was by the authors concluded to be between 15 and 50 mg.kg<sup>-1</sup>. For microorganism nitrification, the NOEC (28-day) was <26 mg.kg<sup>-1</sup>. Thus both the earthworm and the microorganism studies indicate the "true" NOEC in these studies were below 150 and 26 mg.kg<sup>-1</sup>, respectively. The inclusion of cocoon production in the earthworm study and extending the study period to 28 days (short-term studies usually 14 days) may support that the results be considered a long-term study. For microorganisms, longer-term studies tend to result in higher NOECs than short-term studies, whereas the opposite generally applies to studies with multicellular longer living organisms like earthworms. Furthermore, use of long-term test data on microorganisms in the context of effect assessment on soil organisms is presently not explicitly covered by the recommendations given in the TGD. Based on these considerations and since the reported NOEC for nitrification was <26 mg.kg<sup>-1</sup>, 15 mg.kg<sup>-1</sup> from the earthworm study is used in the risk assessment. Thus, based on two long-term studies on plants and earthworm an assessment factor of 50 may be used to reach an indicative PNEC<sub>soil</sub>:*

$$PNEC_{soil} = 15/50 = 0.3 \text{ mg.kg}^{-1}.$$

*For comparison this value is in close agreement with estimation of PNEC employing the equilibrium partitioning method:*

$$PNEC_{soil} = (K_{soil-water}/RHO_{soil}).PNEC_{water.1,000} = 0.26 \text{ mg.kg}^{-1} \text{ w/w.}^?$$

Therefore, the MPC<sub>eco, soil</sub> will be set at a value of 0.3 mg.kg<sup>-1</sup> as well. The value for Dutch standard soil is 0.3\*5.88/2 = 882 µg.kg<sup>-1</sup>.

### 3.1.5.2 MPC<sub>sp, soil</sub>

Toluene has a BCF<100, thus the assessment of secondary poisoning is not triggered.

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

The MPC<sub>human, soil</sub> is based on the TDI of 223  $\mu\text{g}\cdot\text{kg}_{\text{bw}}^{-1}$  (see paragraph 3.1.3.4). 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, mild and meat. Uptake via root crops was determined to be the critical route. The MPC<sub>human, soil</sub> was calculated to be 6.05  $\text{mg}\cdot\text{kg dwt}^{-1}$  Dutch standard soil.

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

The MPC<sub>soil</sub> is equal to the MPC<sub>eco, soil</sub> of 882  $\mu\text{g}\cdot\text{kg}^{-1}$  Dutch standard soil.

### 3.1.5.5 NC<sub>soil</sub>

The NC is set a factor 100 lower compared to the final, integrated MPC<sub>soil</sub>. Thus, the MPC<sub>soil</sub> is 8.82  $\mu\text{g}\cdot\text{kg}^{-1}$  Dutch standard soil.

### 3.1.5.6 SRC<sub>eco, soil</sub>

The geometric mean of the chronic soil data for soil processes is 143  $\text{mg}\cdot\text{kg dw}^{-1}$ . The geometric mean of chronic data for terrestrial single species is 136  $\text{mg}/\text{kg dw}$ . The lowest value of 136  $\text{mg}\cdot\text{kg dw}^{-1}$  is set as SRC<sub>eco, soil</sub>. Thus, the SRC<sub>eco, soil</sub> =  $136 \cdot 5.88/2 = 400 \text{ mg}\cdot\text{kg dw}^{-1}$ .

## 3.1.6 Derivation of ERLs for groundwater

Within the project INS, ecotoxicological ERLs for the groundwater compartment are derived based on ecotoxicological data for the surface-water compartment and on the value for drinking water abstraction.

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

Since groundwater-specific ecotoxicological data are absent, the surface water MPC<sub>eco, water</sub> is taken as substitute. Thus, MPC<sub>eco, gw</sub> = MPC<sub>eco, water</sub> = 74  $\mu\text{g}\cdot\text{l}^{-1}$ .

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

The abstraction of groundwater for use in drinking water is taken into account by using the MPC<sub>dw, water</sub> as MPC<sub>human, gw</sub>. Thus, MPC<sub>human, gw</sub> = MPC<sub>dw, water</sub> = 1730  $\mu\text{g}\cdot\text{l}^{-1}$ . It should be noted, however, that this value exceeds the lowest reported odour threshold in water of 24  $\mu\text{g}\cdot\text{l}^{-1}$  (WHO, 2004).

### 3.1.6.3 Selection of the MPC<sub>gw</sub>

The MPC<sub>gw</sub> is set at the lowest derived value, i.e. 74  $\mu\text{g}\cdot\text{l}^{-1}$ . However, this value exceeds the lowest reported odour threshold value in water of 24  $\mu\text{g}\cdot\text{l}^{-1}$ .

### 3.1.6.4 NC<sub>gw</sub>

The NC<sub>gw</sub> is set a factor 100 lower than the MPC<sub>gw</sub>. Thus, the NC<sub>gw</sub> is  $74/100 = 0.74 \mu\text{g}\cdot\text{l}^{-1}$ .

### 3.1.6.5 SRC<sub>eco, gw</sub>

The SRC<sub>eco, gw</sub> is set equal to SRC<sub>eco, freshw ater</sub>. Thus, the SRC<sub>eco, gw</sub> = 5.7  $\text{mg}\cdot\text{l}^{-1}$ .

### 3.1.7 Toxicity data and derivation of ERLs for air

Due to the high-vapour pressure of toluene the atmosphere is a major recipient of toluene. The photodegradation by photochemical oxidative degradation/ transformation is fast with a half-life of approximately 2 days.

The RAR for toluene reports of the contribution of toluene to ozone formation in the surface near atmosphere and to the formation of other harmful substances such as DNOC. However, the photochemically formation of ozone and other harmful substances in polluted air depend on emission of all VOCs and other compounds in a complex interaction with other factors. In the RAR for toluene, the threshold values for ozone concentrations set in directive 92/72/EEC are summarised, but it is noted that “currently” (i.e. d.d. RAR for toluene) the threshold values are being revised.

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

A number of studies on the effects of toluene in air on plants were summarised in the RAR. It was concluded that toluene did not seem to be of concern with regard to plant toxicity exposed via air, except at very high concentration. No formal PNEC was established because of lack of appropriate long-term studies. However, the NOEC of 60 mg.m<sup>-3</sup> for five plant species after a 14-day exposure period was considered useful to evaluate the risk for terrestrial plants exposed via air.

In analogy with other compartments, an assessment factor of 100 is applied, because the NOEC is derived from one study treating only terrestrial plants. Therefore, an MPC<sub>eco,air</sub> of 600 µg.m<sup>-3</sup> is proposed.

#### 3.1.7.2 MPC<sub>human, air</sub>

In the RAR, the inhalation NOAEC of 1,125 mg.m<sup>-3</sup> of a 2-year study is considered the most relevant for evaluation of effects of long-term exposure in man. The RIVM derived a TCA of 400 µg.m<sup>-3</sup> (Janssen, 1999).

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

The lowest MPC is selected as overall MPC<sub>air</sub>, i.e. 400 µg.m<sup>-3</sup>.

#### 3.1.7.4 NC<sub>air</sub>

The overall MPC<sub>air</sub> divided by 100 is the NC<sub>air</sub>. NC<sub>air</sub> = 4 µg.m<sup>-3</sup>.

## 4 Conclusions

In this report, the risk limits negligible concentration (NC), maximum permissible concentration (MPC), maximum acceptable concentration for ecosystems ( $MAC_{eco}$ ), and serious risk concentration for ecosystems ( $SRC_{eco}$ ) are derived for toluene in water, groundwater, soil and air. No risk limits were derived for the sediment compartment because exposure of sediment is considered negligible. The ERLs that were obtained are summarised in Table 10 below.

**Table 10. Derived MPC, NC,  $MAC_{eco}$ , and  $SRC_{eco}$  values for toluene.**

ERL	Unit	MPC	NC	$MAC_{eco}$	$SRC_{eco}$
Water <sup>a</sup>	$\mu\text{g.l}^{-1}$	74	0.74	550	5,700
Drinking water <sup>a</sup>	$\mu\text{g.l}^{-1}$	1,700			
Marine	$\mu\text{g.l}^{-1}$	7.4	0.07	55 <sup>c</sup>	5,700
Sediment		n.d. <sup>b</sup>			
Soil <sup>d</sup>	$\mu\text{g.kg}_{dw}^{-1}$	880	8.8		$4.0 \times 10^5$
Groundwater	$\mu\text{g.l}^{-1}$	74	0.74		
Air	$\mu\text{g.m}^{-3}$	400	4.0		

<sup>a</sup> The  $MPC_{dw, water}$  is reported as a separate value from the other  $MPC_{water}$  values ( $MPC_{eco, water}$ ,  $MPC_{sp, water}$  or  $MPC_{hh, food, water}$ ). From these other  $MPC_{water}$  values (thus excluding the  $MPC_{dw, water}$ ) the lowest one is selected as the 'overall'  $MPC_{water}$ .

<sup>b</sup> n.d. = not determined.

<sup>c</sup> provisional value.

<sup>d</sup> expressed on Dutch standard soil

## List of abbreviations

ADI	acceptable daily intake
AF	assessment factor
BCF	bioconcentration factor
BMF	biomagnification factor
bw	body weight
CAS	chemical abstract service
d	days
dfi	daily food intake
DG	directorate general
DW	drinking water
DWS	drinking-water standard
EAC	environmentally acceptable concentration
EC	European commission; effect concentration
ECB	European chemicals bureau
ECx	effect concentration at which an effect of x% is observed, generally EC10 and EC50 are calculated
EEC	European economic community (replaced by EU)
EPA	environmental protection agency
EqP	equilibrium partitioning
EQS	environmental quality standard
ERL	environmental risk limit
EU	European union
EU-RAR	European union-risk assessment report
FHI	Fraunhofer Institute
h	hours
INS	International and National Environmental Quality Standards for Substances in the Netherlands (In Dutch: (Inter)nationale Normen Stoffen)
LCx	effect concentration at which x% lethality is observed, generally LC50 and LC10 are calculated
LOEC	lowest observed effect concentration
MAC	maximum acceptable concentration
MATC	maximum acceptable toxicant concentration
NC	negligible concentration
NOEAEC	no observed ecologically adverse effect concentration
NOAEL	no observed adverse effect level
NOEC	no observed effect concentration
NOEL	no observed effect level
oc	organic carbon
om	organic matter
PEC	predicted environmental concentration
PNEC	predicted no effect concentration
QS	quality standard
QSAR	quantitative structure activity relationship
RAR	risk assessment report
RIVM	national institute for public health and the environment
SEC	expertise centre for substances

SMILES	simplified molecular input line entry system
SRC <sub>eco</sub>	ecotoxicological serious risk concentration
STP	sewage treatment plant
susp	suspended particulate matter
TCA	tolerable concentration in air
TDI	tolerable daily intake
TGD	Technical Guidance Document
TL	threshold level
TWA	time weighted average
UV	ultraviolet
VROM	Ministry of Housing, Spatial Planning and the Environment
WFD	water framework directive

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