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## Environmental risk limits for cumene

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## Rapport in het kort

### Milieurisicogrenzen voor cumeen

Dit rapport geeft milieurisicogrenzen voor cumeen (ook vaak cumol genoemd) in (grond)water, bodem en lucht. Milieurisicogrenzen zijn de technisch-wetenschappelijke advieswaarden voor de uiteindelijke milieukwaliteitsnormen in Nederland. De milieurisicogrenzen voor cumeen zijn gebaseerd op de uitkomsten van de EU risicobeoordeling voor cumeen (Bestaande Stoffen Verordening 793/93). De afleiding van de milieurisicogrenzen sluit tevens aan bij de richtlijnen uit de Kaderrichtlijn Water. De beschikbare monitoringsgegevens voor de periode 2003 tot 2006 overschrijden de in dit rapport afgeleide milieurisicogrenzen niet.

Trefwoorden: milieukwaliteitsnormen; milieurisicogrenzen; cumeen; cumol; maximaal toelaatbaar risiconiveau; verwaarloosbaar risiconiveau



# Contents

<b>Summary</b>	<b>8</b>
<b>1 Introduction</b>	<b>9</b>
1.1 Project framework	9
1.2 Production and use of cumene	9
<b>2 Methods</b>	<b>11</b>
2.1 Data collection	11
2.2 Methodology for derivation of environmental risk limits	11
<b>3 Derivation of environmental risk limits for cumene</b>	<b>13</b>
3.1 Substance identification, physico-chemical properties, fate and human toxicology	13
3.2 Trigger values	14
3.3 Toxicity data and derivation of ERLs for water	15
3.4 Toxicity data and derivation of ERLs for sediment	17
3.5 Toxicity data and derivation of ERLs for soil	17
3.6 Derivation of ERLs for groundwater	19
3.7 Derivation of ERLs for air	19
3.8 Comparison of derived ERLs with monitoring data	20
<b>4 Conclusions</b>	<b>21</b>
<b>References</b>	<b>22</b>



## 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 cumene 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 Reports (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.

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.

Available monitoring data for cumene in the Dutch environment for the period 2003-2006 do not exceed the derived ERLs.

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

ERL	unit	value			
		MPC	NC	$MAC_{eco}$	$SRC_{eco}$
water <sup>a</sup>	$\mu\text{g.L}^{-1}$	22	0.22	22	$3.1 \times 10^2$
drinking water <sup>b</sup>	$\text{mg.L}^{-1}$	0.35			
marine	$\mu\text{g.L}^{-1}$	2.2	$2.2 \times 10^{-2}$	2.2	$3.1 \times 10^2$
sediment	$\text{mg.kg}_{dwt}^{-1}$	n.d.			
soil <sup>c</sup>	$\text{mg.kg}_{dwt}^{-1}$	1.2	$1.2 \times 10^{-2}$		16
groundwater	$\mu\text{g.L}^{-1}$	22	0.22		$3.1 \times 10^2$
air	$\text{mg.m}^{-3}$	0.87	$8.7 \times 10^{-3}$		

<sup>a</sup> From the  $MPC_{eco, water}$ ,  $MPC_{sp, water}$  and  $MPC_{hh, food, water}$  the lowest one is selected as the 'overall'  $MPC_{water}$ .

<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>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), soil and groundwater are derived for cumene. 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  $10^{-6}$  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 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 cumene

The Risk Assessment Report (RAR) (European Commission, 2001) states that cumene is produced via alkylation of benzene with propene using an acidic catalyst. From natural sources cumene is manufactured from distillation of coal tar and petroleum fractions. The production volume in the EU ranged between 850 000 and 4 100 000 tonnes in 1992/93. Cumene is used in the chemical industry as basic chemical and for use in synthesis. The compound is mainly used as an intermediate in the production of phenol and acetone. It is also a minor constituent of gasolines and solvents. More details can be found in the RAR (European Commission, 2001).



## 2 Methods

### 2.1 Data collection

The final Risk Assessment Report (RAR) of cumene (European Commission, 2001) produced in the framework of Existing Substances Regulation (793/93/EEC) was used as only source of physico-chemical 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 $MAC_{eco, marine}$

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  $MAC_{eco, water}$  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 cumene

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

##### 3.1.1 Identity

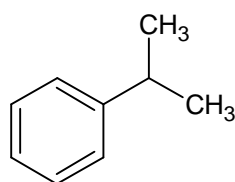


Figure 1. Structural formula of cumene.

Table 2. Identification of cumene.

Parameter	Name or number
Chemical name	cumene
Common/trivial/other name	isopropylbenzene, 1-methyl ethylbenzene, 2-phenylpropane, cumol
CAS number	98-82-8
EC number	202-704-5
Molecular formula:	C <sub>9</sub> H <sub>12</sub>

##### 3.1.2 Physico-chemical properties

Table 3. Physico-chemical properties of cumene.

Parameter	Unit	Value	Remark
Molecular weight	[g.mol <sup>-1</sup> ]	120.19	
Water solubility	[mg.L <sup>-1</sup> ]	50	at 25°C
log <i>K</i> <sub>ow</sub>	[-]	3.55	at 23°C
<i>K</i> <sub>oc</sub>	[L.kg <sup>-1</sup> ]	884	
Vapour pressure	[Pa]	496	at 20°C
Melting point	[°C]	-96	at 1013 hPa
Boiling point	[°C]	152-153	at 1013 hPa
Henry's law constant	[Pa.m <sup>3</sup> .mol <sup>-1</sup> ]	1010.8	at 20°C

### 3.1.3 Behaviour in the environment

Table 4. Selected environmental properties of cumene.

Parameter	Unit	Value	Remark	Reference
Hydrolysis half-life	DT50 [h]	5.1		RAR
Photolysis half-life	DT50 [d]	2.4		RAR
Degradability		inherently biodegradable		RAR

### 3.1.4 Bioconcentration and biomagnification

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

Table 5. Overview of bioaccumulation data for cumene.

Parameter	Unit	Value	Remark	Reference
BCF (fish)	[L.kg <sup>-1</sup> ]	208 and 224	calculated	RAR
BMF	[kg.kg <sup>-1</sup> ]	1	Default value since the BCF is less than 2000 L.kg <sup>-1</sup>	

### 3.1.5 Human toxicology: classification and limit values

Classification and labelling according to the 25<sup>th</sup> ATP of Directive 67/548/EEC:

Classification: R10, R37, R51/53 and R65. Labelling: Xn, Xi, N

The RAR concludes cumene is not genotoxic based on available evidence. Carcinogenicity data are lacking (considered of low priority given the negative genotoxicity). In the RAR an oral NOAEL of 154 mg.kg<sub>bw</sub><sup>-1</sup>day<sup>-1</sup> from a 6-months rat study was selected as overall-NOAEL for repeated dose toxicity. For inhalation the overall NOAEL was 490 mg/m<sup>3</sup> taken from a 90-day inhalation study in rats. Existing limit values as derived by US-EPA and RIVM are in agreement with these NOAELs. The US-EPA (2000) derived an RfD of 0.1 mg.kg<sub>bw</sub><sup>-1</sup>day<sup>-1</sup> based on the NOAEL of 154 mg/kg<sub>bw</sub>/day (the same oral NOAEL as selected in the RAR). RIVM derived an inhalation limit value (TCA) of 870 µg.m<sup>-3</sup> based on the inhalation NOAEL of 490 mg/m<sup>3</sup> (the same inhalation NOAEL as selected in the RAR) (Dusseldorp et al. 2004). The limit values of RIVM and US-EPA will be used in the present report.

## 3.2 Trigger values

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

Table 6. Cumene: collected properties for comparison to MPC triggers.

Parameter	Value	Unit	Method/Source
Log $K_{p,susp-water}$	1.9	[-]	$K_{OC} \times f_{OC,susp}^1$
BCF	216	[L.kg <sup>-1</sup> ]	average of 208 and 224
BMF	1	[kg.kg <sup>-1</sup> ]	
Log $K_{OW}$	3.55	[-]	
R-phrases	10, 37, 51/53, 65	[-]	
A1 value	-	[µg.L <sup>-1</sup> ]	
DW standard	-	µg.L <sup>-1</sup> ]	

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

- cumene has a  $\log K_{p, \text{susp-water}} < 3$ ; derivation of  $\text{MPC}_{\text{sediment}}$  is not triggered.
- cumene has a  $\log K_{p, \text{susp-water}} < 3$ ; expression of the  $\text{MPC}_{\text{water}}$  as  $\text{MPC}_{\text{susp, water}}$  is not required.
- cumene has a  $\log K_{\text{ow}} > 3$ ; assessment of secondary poisoning is triggered.
- cumene has no R classification for which an  $\text{MPC}_{\text{water}}$  for human health via food (fish) consumption ( $\text{MPC}_{\text{hh food, water}}$ ) should be derived.

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

An overview of the selected freshwater toxicity data for cumene, excluding the low quality data, as reported in the RAR is given in Table 7 and marine toxicity data are shown in Table 8.

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

<b>Chronic</b> <b>Taxonomic group</b>	<b>NOEC/EC<sub>10</sub> (mg.L<sup>-1</sup>)</b>	<b>Acute</b> <b>Taxonomic group</b>	<b>L(E)C<sub>50</sub> (mg.L<sup>-1</sup>)</b>
<b>Bacteria</b>		<b>Bacteria</b>	
		<i>Pseudomonas putida</i>	211
<b>Algae</b>		<b>Algae</b>	
<i>Scenedesmus subspicatus</i>	<b>0.22</b>	<i>Chlorella vulgaris</i>	21.27
		<i>Chlamydomonas angulosa</i>	8.8
		<i>Pseudokirchneriella subcapitata</i>	2.6
		<b>Protozoa</b>	
		<i>Dicranophorus forcipatus</i>	172
<b>Crustacea</b>		<b>Crustacea</b>	
<i>Daphnia magna</i>	0.35	<i>Daphnia magna</i>	3.0*
<b>Pisces</b>		<b>Pisces</b>	
Fish (QSAR)	0.38	<i>Oncorhynchus mykiss</i>	3.6**
		<i>Poecilia reticulata</i>	5.1

The value in bold is used for derivation of the MPC.

\* Geometric mean of all 48h EC50 values reported in the RAR: 10.8, 0.6, 4.

\*\* Geometric mean of 4.8 and 2.7 mg.L<sup>-1</sup>.

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

<b>Chronic</b> <b>Taxonomic group</b>	<b>NOEC/EC<sub>10</sub> (mg.L<sup>-1</sup>)</b>	<b>Acute</b> <b>Taxonomic group</b>	<b>L(E)C<sub>50</sub> (mg.L<sup>-1</sup>)</b>
<b>Crustacea</b>		<b>Crustacea</b>	
		<i>Artemia salina</i>	7.3
		<i>Americamysis bahia</i>	<b>1.3</b>
<b>Pisces</b>		<b>Pisces</b>	
		<i>Cypridon variegatus</i>	4.7

The value in bold is used for derivation of the MAC.

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

There is no complete dataset available for marine species and in the RAR freshwater and marine data are pooled. Therefore in this report data for freshwater and marine species are pooled as well.



### 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>

In the RAR a PNEC of 22 µg.L<sup>-1</sup> for aquatic organisms has been derived based on the NOEC of 0.22 mg.L<sup>-1</sup> for *Scenedesmus subspicatus*. A factor of 10 has been used since chronic data for 3 trophic levels are available, the QSAR for fish was included. The MPC<sub>eco, water</sub> will be set equal to the PNEC. The MPC<sub>eco, water</sub> is: 22 µg.L<sup>-1</sup>.

In the RAR it is stated that the PNEC derived is also to be used for marine environments. However, considering the data available the marine MPC should be derived with an assessment factor of 100 since no chronic data are available for marine species. Therefore the MPC<sub>eco, marine</sub> will be: 2.2 µg.L<sup>-1</sup>.

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

Cumene has a BCF > 100 L.kg<sup>-1</sup>, thus assessment of secondary poisoning is triggered.

Table 9. Cumene: selected bird and mammal data for ERL derivation.

Species	Exposure time	Criterion	Effect concentration (mg.kg <sub>diet</sub> <sup>-1</sup> )	Assessment factor	MPC <sub>oral</sub> (mg.kg <sub>diet</sub> <sup>-1</sup> )
Rat	6 months	NOEC	3080	30	102.7

The NOEC reported above has been calculated in the RAR from the chronic NOAEL of 154 mg.kg<sub>bw</sub><sup>-1</sup>.day<sup>-1</sup> for rats. As reported in Van Vlaardingen and Verbruggen (2007) this value can be converted into a NOEC using a conversion factor of 20: 154\*20 = 3080 mg/kg diet. With an assessment factor of 30 as used for chronic exposed mammals, the MPC<sub>oral</sub> will be 102.7 mg/kg diet. The MPC<sub>sp, water</sub> is then: MPC<sub>oral</sub>/ BCF<sub>fish</sub>\*BMF: 102.7/ (216\*1) = 0.48 mg.L<sup>-1</sup>.

The MPC<sub>sp, marine</sub> is calculated with an extra BMF<sub>2</sub> of 1 and becomes 102.7 / (216\*1\*1) = 0.48 mg.L<sup>-1</sup>.

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

Derivation of MPC<sub>hh food, water</sub> for cumene is not triggered (Table 6).

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

The MPC<sub>eco, water</sub> is the lowest MPC<sub>water</sub> derived. Therefore the MPC water is 22 µg.L<sup>-1</sup>.

The MPC<sub>marine</sub> is the MPC<sub>eco, marine</sub>: 2.2 µg.L<sup>-1</sup>.

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

No A1 value and DW standard are available for cumene. With the RfD of 0.1 mg.kg<sub>bw</sub><sup>-1</sup>.day<sup>-1</sup> 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 the TL<sub>hh</sub> is the RfD, 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 \* 0.1 \* 70 / 2 = 0.35 mg.L<sup>-1</sup>.

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

The MAC<sub>eco</sub> is to be based on the lowest L(E)C50 available (1.3 mg.L<sup>-1</sup> for *Pseudokirchneriella subcapitata*). The assessment factor to be applied is 1000 since cumene has a potential to

bioaccumulate, a  $\log K_{ow} > 3$ , a non-specific mode of action (narcosis) and a high interspecies variation. Therefore the  $MAC_{eco}$  is initially set to  $1.3/1000 = 1.3 \mu\text{g.L}^{-1}$ . This value is lower than the  $MPC_{eco, water}$  of  $22 \mu\text{g.L}^{-1}$ . 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, the  $MAC_{eco, water}$  is set equal to the  $MPC_{eco, water}$ :  $22 \mu\text{g.L}^{-1}$ .

An additional assessment factor of 5 is used for the  $MAC_{eco, marine}$  because there is acute toxicity data for one additional marine taxonomic group, *Cypridon variegatus*. The two crustacea in Table 8 do not account as an additional marine taxonomic group since they have the same life form and feeding strategy as freshwater crustacea like *Daphnia* sp. The  $MAC_{eco, marine}$  is  $1.3 / 1000 / 5 = 0.26 \mu\text{g.L}^{-1}$ . Since this value is lower than the  $MPC_{eco, marine}$  of  $2.2 \mu\text{g.L}^{-1}$ , the  $MAC_{eco, marine}$  is set equal to the  $MPC_{eco, marine}$ :  $2.2 \mu\text{g.L}^{-1}$ . It has to be noted that this procedure for the  $MAC_{eco, marine}$  is currently not agreed upon. Therefore the  $MAC_{eco, marine}$  needs to be re-evaluated once an agreed procedure is available.

### 3.3.6 Derivation of NC

The  $NC_{water}$  is set a factor of 100 below the  $MPC_{water}$ . Therefore the  $NC_{water}$  is  $22/100 = 0.22 \mu\text{g.L}^{-1}$ . The  $NC_{marine}$  is  $2.2/100 = 0.022 \mu\text{g.L}^{-1}$ .

### 3.3.7 Derivation of $SRC_{eco, aquatic}$

For derivation of the  $SRC_{eco, aquatic}$  both chronic and acute data are available as presented in Table 7. The geometric mean of the acute values divided by 10 ( $1.3 \text{ mg.L}^{-1}$ ) is higher than the geometric mean of the chronic values ( $0.31 \text{ mg.L}^{-1}$ ). Therefore the  $SRC_{eco, aquatic}$  is the geometric mean of all chronic values with an assessment factor of 1:  $0.31/1 = 0.31 \text{ mg.L}^{-1}$ . The  $SRC_{eco, aquatic}$  is valid for the marine and the freshwater environment.

## 3.4 Toxicity data and derivation of ERLs for sediment

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

## 3.5 Toxicity data and derivation of ERLs for soil

An overview of the selected soil toxicity data for cumene is given in Table 10.

Table 10. Cumene: selected soil data for ERL derivation.

Chronic		Acute	
Taxonomic group	NOEC/EC10 ( $\text{mg.kg}_{dwt}^{-1}$ )	Taxonomic group	L(E)C50
<i>Helianthus annuus</i>	$\geq 1000$		
<i>Phaseolus aureus</i>	$\geq 1000$		
<i>Sorgum bicolour</i>	$\geq 1000$		

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

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

In the RAR, the data presented in Table 10 were considered not suitable to derive a PNEC since these results were only unbound values based on the highest test concentration of 1000 mg.kg<sub>dwt</sub><sup>-1</sup>. Therefore a PNEC was derived using the equilibrium partitioning method. The PNEC<sub>terrestrial organisms</sub> obtained in the RAR was 0.347 mg.kg<sub>wwt</sub><sup>-1</sup>. Conversion to Dutch standard soil and dry weight soil gives an MPC<sub>eco, soil</sub> of 1.16 mg.kg<sub>dwt</sub><sup>-1</sup>.

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

Cumene has a BCF > 100 L.kg<sup>-1</sup> and therefore secondary poisoning is triggered. The MPC<sub>sp, soil</sub> can be calculated from the MPC<sub>oral</sub> of 102.7 mg.kg<sub>diet</sub><sup>-1</sup> as given in table 9. The MPC<sub>sp, soil, TGD</sub> can be calculated with the following formula:

$$MPC_{sp, soil, TGD} = \frac{MPC_{oral, min} \cdot (1 + F_{gut} \cdot CONV_{soil})}{BCF_{earthworm} \cdot \frac{RHO_{soil}}{K_{soil-water} \cdot CONV_{soil} \cdot 1000} + F_{gut}}$$

The BCF<sub>earthworm</sub> has been calculated with the QSAR:

$$BCF_{earthworm} = 0.84 + \frac{0.012 \cdot K_{OW}}{RHO_{earthworm}}$$

The following defaults are used:

F <sub>gut</sub>	0.1	kg <sub>dw</sub> .kg <sub>ww</sub> <sup>-1</sup>
RHO <sub>soil</sub>	1.7	kg <sub>wwt</sub> .L <sup>-1</sup>
RHO <sub>earthworm</sub>	1	kg <sub>wwt</sub> .L <sup>-1</sup>
CONV <sub>soil</sub>	1.13	kg <sub>ww</sub> .kg <sub>dwt</sub> <sup>-1</sup>
K <sub>soil-water</sub>	28	m <sup>3</sup> .m <sup>-3</sup>

The calculated MPC<sub>sp, soil, TGD</sub> is: 45.2 mg/kg<sub>dwt</sub>. Conversion to Dutch standard soil gives: 132.9 mg.kg<sub>dwt st soil</sub><sup>-1</sup>.

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

For the derivation of the MPC<sub>human, soil</sub>, the US-EPA RfD of 0.1 mg.kg<sub>bw</sub><sup>-1</sup>.day<sup>-1</sup> can be used as TL<sub>hh</sub> with the method as described in van Vlaardingen and Verbruggen (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, mild and meat. Uptake via root crops was determined to be the critical route. The calculated MPC<sub>human, soil</sub> is 1.86 mg.kg<sub>dwt</sub><sup>-1</sup> for Dutch standard soil.

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

The lowest MPC<sub>soil</sub> is the MPC<sub>eco, soil</sub>: 1.16 mg.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<sub>soil</sub> of 11.6 µg.kg<sub>dwt</sub><sup>-1</sup> for Dutch standard soil.

### 3.5.3 Derivation of $\text{SRC}_{\text{eco, soil}}$

The equilibrium partitioning method can be used to calculate an  $\text{SRC}_{\text{eco, soil}}$  from the  $\text{SRC}_{\text{eco, aquatic}}$  ( $0.31 \text{ mg.L}^{-1}$ ). This method gives an  $\text{SRC}_{\text{eco, soil, dwt}}$  of  $5.5 \text{ mg.kg}_{\text{dwt}}^{-1}$ . Conversion to Dutch standard soil gives an  $\text{SRC}_{\text{eco, soil}}$  of:  $16.3 \text{ mg.kg}_{\text{dwt}}^{-1}$ .

## 3.6 Derivation of ERLs for groundwater

### 3.6.1 Derivation of $\text{MPC}_{\text{gw}}$

#### 3.6.1.1 $\text{MPC}_{\text{eco, gw}}$

Since groundwater-specific ecotoxicological ERLs for the groundwater compartment are absent, the surface water  $\text{MPC}_{\text{eco, water}}$  is taken as a substitute. Thus, the  $\text{MPC}_{\text{eco, gw}} = \text{MPC}_{\text{eco, water}} = 22 \text{ }\mu\text{g.L}^{-1}$ .

#### 3.6.1.2 Derivatisation of $\text{MPC}_{\text{human, gw}}$

The  $\text{MPC}_{\text{human, gw}}$  is set equal to the  $\text{MPC}_{\text{dw, water}}$  of  $0.35 \text{ mg.L}^{-1}$ .

#### 3.6.1.3 Selection of the $\text{MPC}_{\text{gw}}$

The lowest  $\text{MPC}_{\text{gw}}$  is the  $\text{MPC}_{\text{eco, gw}}$  of  $22 \text{ }\mu\text{g.L}^{-1}$ . Thus, the final  $\text{MPC}_{\text{gw}} = 22 \text{ }\mu\text{g.L}^{-1}$ .

### 3.6.2 Derivation of $\text{NC}_{\text{gw}}$

The  $\text{NC}_{\text{gw}}$  is set a factor of 100 lower than the  $\text{MPC}_{\text{gw}}$ . Thus,  $\text{NC}_{\text{gw}} = 22/100 = 0.22 \text{ }\mu\text{g.L}^{-1}$ .

### 3.6.3 Derivation of $\text{SRC}_{\text{eco, gw}}$

The  $\text{SRC}_{\text{eco, gw}}$  is set equal to  $\text{SRC}_{\text{eco, aquatic}}$ . Thus, the  $\text{SRC}_{\text{eco, gw}} = 0.31 \text{ mg.L}^{-1}$ .

## 3.7 Derivation of ERLs for air

### 3.7.1 Derivation of $\text{MPC}_{\text{air}}$

#### 3.7.1.1 $\text{MPC}_{\text{eco, air}}$

The RAR reports that no ecotoxicological data are available for the atmospheric compartment. Therefore no  $\text{MPC}_{\text{eco, air}}$  can be derived.

#### 3.7.1.2 Derivation of $\text{MPC}_{\text{human, air}}$

A TCA for cumene of  $870 \text{ }\mu\text{g.m}^{-3}$  has been derived by Dusseldorp *et al.* (2004), this value will set the  $\text{MPC}_{\text{human, air}}$ . Therefore the  $\text{MPC}_{\text{human, air}}$  will be  $870 \text{ }\mu\text{g.m}^{-3}$ .

#### 3.7.1.3 Selection of the $\text{MPC}_{\text{air}}$

The only  $\text{MPC}_{\text{air}}$  derived is the  $\text{MPC}_{\text{human, air}}$ , therefore the  $\text{MPC}_{\text{air}}$  is set to the  $\text{MPC}_{\text{human, air}}$ :  $870 \text{ }\mu\text{g.m}^{-3}$ .

### 3.7.2 Derivation of $\text{NC}_{\text{air}}$

The  $\text{MPC}_{\text{air}}$  divided by 100 is the  $\text{NC}_{\text{air}}$ :  $8.7 \text{ }\mu\text{g.m}^{-3}$ .

### 3.8 Comparison of derived ERLs with monitoring data

The monitoring data for cumene reported by the RIWA (Dutch Association of River Water companies, [www.riwa.org](http://www.riwa.org)) for the years 2003 to 2006 shows that the monthly average concentrations of cumene in the Rhine were always below the level of detection ( $0.03 \mu\text{g}\cdot\text{L}^{-1}$ ). This value is below the MPCs derived for the water compartments.

## 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 cumene 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 the table below. Available monitoring data for cumene in the Dutch environment for the period 2003-2006 do not exceed the derived ERLs.

Table 11. Derived MPC, NC,  $MAC_{eco}$ , and  $SRC_{eco}$  values for cumene.

ERL	unit	value			
		MPC	NC	$MAC_{eco}$	$SRC_{eco}$
water <sup>a</sup>	$\mu\text{g.L}^{-1}$	22	0.22	22	$3.1 \times 10^2$
drinking water <sup>b</sup>	$\text{mg.L}^{-1}$	0.35			
marine	$\mu\text{g.L}^{-1}$	2.2	$2.2 \times 10^{-2}$	2.2	$3.1 \times 10^2$
sediment	$\text{mg.kg}_{dwt}^{-1}$	n.d.			
soil <sup>c</sup>	$\text{mg.kg}_{dwt}^{-1}$	1.2	$1.2 \times 10^{-2}$		16
groundwater	$\mu\text{g.L}^{-1}$	22	0.22		$3.1 \times 10^2$
air	$\text{mg.m}^{-3}$	0.87	$8.7 \times 10^{-3}$		

<sup>a</sup> From the  $MPC_{eco, water}$ ,  $MPC_{sp, water}$  and  $MPC_{hh \text{ food, water}}$  the lowest one is selected as the 'overall'  $MPC_{water}$ .

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

n.d. = not derived.

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