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Environmental risk limits for benzene, C10-13 alkyl derives. (LAB)

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Rapport in het kort

Milieurisicogrenzen voor lineaire C₁₀-C₁₃ alkylbenzenen (LAB)

Dit rapport geeft milieurisicogrenzen voor lineaire C₁₀-C₁₃ alkylbenzenen (LAB) in (grond)water, sediment, bodem en lucht. Milieurisicogrenzen zijn de technisch-wetenschappelijke advieswaarden voor de uiteindelijke milieukwaliteitsnormen in Nederland. De milieurisicogrenzen voor LAB zijn gebaseerd op de uitkomsten van de EU risicobeoordeling voor LAB (Bestaande Stoffen Verordening 793/93). De afleiding van de milieurisicogrenzen sluit tevens aan bij de richtlijnen uit de Kaderrichtlijn Water. Monitoringsgegevens voor Nederland zijn niet beschikbaar, daarom kan er geen verwachting worden uitgesproken of de afgeleide milieurisicogrenzen in Nederland overschreden zullen worden.

Trefwoorden: milieukwaliteitsnormen; milieurisicogrenzen; lineaire C₁₀-C₁₃ alkylbenzenen; LAB; benzeen, C10-13 alkylderivaten; 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 LAB in water, groundwater, sediment, 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).

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 LAB 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_{eco} , and SRC_{eco} values for LAB.

| ERL | unit | value | NC | MAC_{eco} | SRC_{eco} |
|-----------------------------------|-----------------------------|----------------------|----------------------|----------------------|-------------------|
| | | MPC | | | |
| water ^a | $\mu\text{g.L}^{-1}$ | 0.75 | 7.5×10^{-3} | 0.75 | 2.7 |
| water susp. matter. ^c | mg.kg_{dwt}^{-1} | 1.8 | | | |
| drinking water ^b | mg.L^{-1} | 0.88 | | | |
| marine | $\mu\text{g.L}^{-1}$ | 7.5×10^{-2} | 7.5×10^{-4} | 7.5×10^{-2} | 2.7 |
| marine susp. matter. ^c | mg.kg_{dwt}^{-1} | 0.19 | | | |
| water, sediment ^d | mg.kg_{dwt}^{-1} | 0.97 | 9.7×10^{-3} | | 3.5 |
| marine, sediment ^d | mg.kg_{dwt}^{-1} | 9.7×10^{-2} | 9.7×10^{-4} | | 3.5 |
| soil ^e | $\mu\text{g.kg}_{dwt}^{-1}$ | 2.1 | 2.1×10^{-2} | | 3.5×10^3 |
| groundwater | $\mu\text{g.L}^{-1}$ | 0.75 | 7.5×10^{-3} | | 2.7 |
| air | $\mu\text{g.m}^{-3}$ | 90 | 0.90 | | |

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

^b 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.

^c Expressed on the basis of Dutch standard suspended matter.

^d Expressed on the basis of Dutch standard sediment.

^e Expressed on the basis of Dutch standard soil.

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 LAB. 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 LAB

The Risk Assessment Report (RAR) (EC, 1999) reports that LAB is almost entirely (>99%) utilised as intermediate in the production of Linear Alkylbenzene Sulfonates (LAS). Some LAB also finds minor use as solvent and binder in speciality applications, e.g. cable oil, ink industry, paint and varnishes, insulating and electricity. In 1995 the LAB production in Western Europe was estimated at 450 ktonnes a year. Consumption in Western Europe was estimated at 280 ktonnes a year. More details can be found in the RAR (EC, 1999).

2 Methods

2.1 Data collection

The final Risk Assessment Report (RAR) of LAB (EC, 1999) 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:

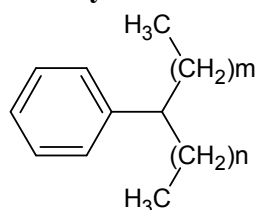
- the assessment factor for the $MAC_{eco, water}$ value, when acute toxicity data for at least two specific marine taxa are available, or
- using an additional assessment factor of 5, when acute toxicity data for only one specific marine taxon are available (analogous to the derivation of the MPC according 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 LAB

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

3.1.1 Identity



(m + n = 7 to 10)

Figure 1. Structural formula of LAB.

Table 2. Identification of LAB.

| Parameter | Name or number |
|---------------------------|--|
| Chemical name | Benzene, C ₁₀₋₁₃ alkyl derivatives |
| Common/trivial/other name | Linear alkylbenzene, LAB |
| CAS number | 67774-74-7 |
| EC number | 267-051-0 |
| Molecular formula: | C ₆ H ₅ C _n H _{2n+1} n = 10 - 13 |
| SMILES code | CCCCC(CCCCCC)c1ccccc1 example for one isomer |

3.1.2 Physico-chemical properties

Table 3. Physico-chemical properties of LAB.

| Parameter | Unit | Value | Remark |
|---------------------|---|-----------------------|---|
| Molecular weight | [g.mol ⁻¹] | 239-243 | This is an average weight of the mixture. The weight of the individual isomers ranges from 218 to 260 g.mol ⁻¹ . |
| Water solubility | [mg.L ⁻¹] | 0.041 | |
| log K _{ow} | [-] | 7.5-9.12 | calculated, 25°C, the mean, 8.3, is used in this report |
| K _{oc} | [L.kg ⁻¹] | 2.2 x 10 ⁴ | measured in 4 types of soil |
| Vapour pressure | [Pa] | 1.3 | At 25°C |
| | | 399 | At 300°C |
| Melting point | [°C] | < -70 | |
| Boiling range | [°C] | 278-314 | |
| Henry's constant | [Pa.m ³ .mol ⁻¹] | 95 | |

In the RAR an explanation is not always given on how one value is derived for a mixture of compounds.

3.1.3 Behaviour in the environment

Table 4. Selected environmental properties of LAB.

| Parameter | Unit | Value | Remark | Reference |
|----------------------|----------|---------|----------------------------------|-----------|
| Hydrolysis half-life | DT50 [d] | n.a. | | |
| Photolysis half-life | DT50 [d] | | No significant direct photolysis | EC, 1999 |
| Degradability | | readily | | EC, 1999 |

n.a. = not available

3.1.4 Bioconcentration and biomagnification

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

Table 5. Overview of bioaccumulation data for LAB.

| Parameter | Unit | Value | Remark | Reference |
|------------|------------------------|-------|--|-----------|
| BCF (fish) | [L.kg ⁻¹] | 35 | measured | EC, 1999 |
| BMF | [kg.kg ⁻¹] | 1 | default value since the BCF <2000 L.kg ⁻¹ . | |

According to the RAR (EC, 1999), the log K_{ow} of 7.5 – 9.1 would predict a potentially high bioaccumulation in fish. However, the measured BCF of 35 in a test with *Lepomis macrochirus* is thought to imply low bioconcentration potential. In the RAR, it is postulated that this can be explained by the high rate of metabolism of LAB by the fish. In the RAR, several clues are suggested. First, the rates of uptake and depuration of chemicals which are highly degradable are different from the rates of chemicals, which persist in biological tissue. Persistent chemicals have slow, continued uptake and extremely retarded depuration with half-lives extending to 100 days. In contrast, the uptake time of 90% steady state whole fish concentration was less than a week and the time to clear 50% of the steady state whole fish concentration was two days. Furthermore, similarities are found in the uptake and depuration kinetics data for LAB and its sulphonated derivative LAS, which is known to be metabolised. This situation may indicate that the chemical is metabolised in the liver and eliminated via biliary excretion and in the urine. This interpretation is thought to be supported by the findings from studies conducted on radiolabelled LAB to determine its distribution, metabolism and excretion in warm-blooded animals.

3.1.5 Human toxicology: classification and limit values

Classification and labeling according to the 25th ATP of Directive 67/548/EEC:

Classification: R50

Labelling: N

The data as presented in the RAR show that LAB has limited oral and inhalation toxicity. RIVM/SIR has derived the inhalation limit value (Tolerable Concentration in Air, TCA) using the inhalation NOAEL of 102 mg.m⁻³ taken from a 14 weeks inhalation study with rats reported as overall NOAEL for repeated-dose toxicity in the RAR. The NOAEL was corrected for exposure time from 30 to 168 hours a week and an assessment factor of 200 was applied (an assessment factor of 10 for extrapolation from testing animal to human; an assessment factor of 10 for extrapolation to sensitive groups; and an assessment factor of 2 for extrapolation from subchronic to chronic). The derived TCA is: 90 µg.m⁻³.

For derivation of the oral limit value (Tolerable Daily Intake, TDI), the reproduction NOAEL of $50 \text{ mg.kg}_{\text{bw}}^{-1}.\text{day}^{-1}$ reported in the RAR was used. This value originated from a two-generation rat study on reproduction toxicity. On this NOAEL an assessment factor of 200 was applied (an assessment factor of 10 for extrapolation from testing animal to human; an assessment factor of 10 for extrapolation to sensitive groups; and an assessment factor of 2 for extrapolation for limited duration of the study used). The derived TDI is $250 \text{ }\mu\text{g.kg}_{\text{bw}}^{-1}.\text{day}^{-1}$.

3.2 Trigger values

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

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

| Parameter | Value | Unit | Method/Source |
|---------------------------------------|----------|------------------------|---|
| $\text{Log } K_{\text{p,susp-water}}$ | 3.3 | [-] | $K_{\text{OC}} \times f_{\text{OC,susp}}^1$ |
| BCF | 35 | $[\text{L.kg}^{-1}]$ | |
| BMF | 1 | $[\text{kg.kg}^{-1}]$ | |
| $\text{Log } K_{\text{OW}}$ | 7.5-9.12 | [-] | |
| R-phrases | 50 | [-] | |
| A1 value | - | $[\mu\text{g.L}^{-1}]$ | |
| DW standard | - | $[\mu\text{g.L}^{-1}]$ | |

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

- LAB has a $\text{log } K_{\text{p,susp-water}} > 3$; derivation of $\text{MPC}_{\text{sediment}}$ is triggered.
- LAB has a $\text{log } K_{\text{p,susp-water}} > 3$; expression of the $\text{MPC}_{\text{water}}$ as $\text{MPC}_{\text{susp, water}}$ is required.
- LAB has a $\text{BCF} < 100 \text{ L.kg}^{-1}$; assessment of secondary poisoning is not triggered.
- LAB 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

3.3.1 $\text{MPC}_{\text{eco, water}}$ and $\text{MPC}_{\text{eco, marine}}$

An overview of the selected freshwater toxicity data for LAB as reported in the RAR is given in Table 7 and marine toxicity data are shown in Table 8.

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

| Chronic | | Acute | |
|--|---|---------------------------|---|
| Taxonomic group | NOEC/EC ₁₀ (mg.L ⁻¹) | Taxonomic group | L(E)C ₅₀ (mg.L ⁻¹) |
| Algae | | Bacteria | |
| <i>Pseudokirchneriella subcapitata</i> | NOEC>solubility | <i>Pseudomonas putida</i> | EC10>solubility |
| | | <i>Pseudomonas putida</i> | EC10>solubility |
| Crustacea | | Crustacea | |
| <i>Daphnia magna</i> | 0.0075 | <i>Daphnia magna</i> | 0.009-0.08 |
| | | <i>Daphnia magna</i> | NOEC>solubility |
| | | <i>Americamysis bahia</i> | NOEC>solubility |
| | | <i>Gammarus fasciatus</i> | NOEC>solubility |

| Chronic Taxonomic group | NOEC/EC ₁₀ (mg.L ⁻¹) | Acute Taxonomic group | L(E)C ₅₀ (mg.L ⁻¹) |
|----------------------------|---|---------------------------------|---|
| | | <i>Paratanytarsus spec.</i> | NOEC>solubility |
| | | Pisces | |
| | | <i>Leuciscus idus melanotus</i> | NOEC>solubility |
| | | <i>Lepomis macrochirus</i> | NOEC>solubility |
| | | <i>Pimephales promelas</i> | NOEC>solubility |
| | | <i>Onchorhynchus mykiss</i> | NOEC>solubility |

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

| Chronic Taxonomic group | NOEC/EC ₁₀ (mg.L ⁻¹) | Acute Taxonomic group | L(E)C ₅₀ (mg.L ⁻¹) |
|----------------------------|---|-------------------------------|---|
| | | Crustacea | |
| | | <i>Chaetogammarus marinus</i> | >solubility (NOEC) |

3.3.2 Treatment of fresh- and saltwater toxicity data

Freshwater and saltwater data are combined because there are data for only one marine species.

3.3.3 Mesocosm studies

No mesocosm studies are presented in the RAR.

3.3.4 Derivation of MPC_{water} and MPC_{marine}

3.3.4.1 MPC_{eco, water} and MPC_{eco, marine}

In the RAR most studies presented were performed at concentrations higher than the water solubility. Nevertheless a PNEC has been derived using the only chronic value available which was 7.5 µg.L⁻¹ for *Daphnia magna*. This value was below the water solubility. Since the RAR considered the algae test, a 4-day test covering several generations, a chronic test, there are two chronic tests available. *Daphnia* is the most sensitive species in the acute studies and in the RAR is also stated that it is highly probable that *Daphnia* is the most sensitive species in the chronic studies. Considering these facts and the low BCF (35 L.kg⁻¹), an assessment factor of 10 has been applied. Therefore the PNEC_{surface water} derived in the RAR is 0.75 µg.L⁻¹. The MPC_{eco, water} is set equal to the PNEC_{surface water} as derived in the RAR and is: 0.75 µg.L⁻¹.

For derivation of the MPC_{eco, marine}, the same *Daphnia* study can be used and based on the same arguments as used for the PNEC_{surface water} an assessment factor of 100 can be applied. The MPC_{eco, marine} is 7.5 / 100 = 0.075 µg.L⁻¹.

3.3.4.2 MPC_{sp, water} and MPC_{sp, marine}

LAB has a BCF < 100 L.kg⁻¹, thus assessment of secondary poisoning is not triggered.

3.3.4.3 MPC_{hh food, water}

Derivation of MPC_{hh food, water} for LAB is not triggered (Table 6).

3.3.4.4 Selection of the MPC_{water} and MPC_{marine}

The only MPC_{water} derived is the MPC_{eco, water}. Therefore, the MPC_{water} is the MPC_{eco, water}: 0.75 µg.L⁻¹. The MPC_{marine} is the MPC_{eco, marine}: 0.075 µg.L⁻¹.

Since LAB has a $K_{p, \text{susp-water}} \geq 3$ the $\text{MPC}_{\text{water}}$ should also be expressed as $\text{MPC}_{\text{susp, water}}$. The $\text{MPC}_{\text{susp, water}}$ is calculated according to:

$$\text{MPC}_{\text{susp, water}} = \text{MPC}_{\text{water, total}} / (C_{\text{susp, Dutch standard}} \times 10^{-6} + (1 / K_{p, \text{susp-water, Dutch standard}}))$$

For this calculation, $K_{p, \text{susp-water, Dutch standard}}$ is calculated from the $K_{p, \text{susp-water}}$ as calculated in the RAR based on a $f_{\text{OC, susp}}$ of 0.1. This is the same as the European standard $f_{\text{OC, susp}}$ which is used in the table with trigger values. With an $f_{\text{OC, susp, Dutch standard}}$ of 0.1176 the $K_{p, \text{susp-water, Dutch standard}}$ can be recalculated to 2587 L.kg^{-1} . With this value and a $C_{\text{susp, Dutch standard}}$ of 30 mg.L^{-1} the $\text{MPC}_{\text{susp, water}}$ is: $1.8 \text{ mg.kg}_{\text{dwt}}^{-1}$.

The $\text{MPC}_{\text{susp, marine}}$ is calculated in a similar way from the $\text{MPC}_{\text{marine}}$ and a $C_{\text{susp, marine}}$ of 3 mg.L^{-1} at $0.19 \text{ mg.kg}_{\text{dwt}}^{-1}$.

3.3.5 $\text{MPC}_{\text{dw, water}}$

No A1 value and DW standard are available for LAB. With the ADI of $250 \text{ } \mu\text{g.kg}_{\text{bw}}^{-1}.\text{d}^{-1}$ an $\text{MPC}_{\text{dw, water, provisional}}$ can be calculated with the following formula:

$\text{MPC}_{\text{dw, water, provisional}} = 0.1 \cdot \text{TL}_{\text{hh}} \cdot \text{BW} / \text{Uptake}_{\text{dw}}$ where the TL_{hh} is the ADI, BW is a body weight of 70 kg, and $\text{uptake}_{\text{dw}}$ is a daily uptake of 2 L. As described in section 2.2 water treatment is currently not taken into account. Therefore the $\text{MPC}_{\text{dw, water}} = \text{the MPC}_{\text{dw, water, provisional}}$ and becomes:
 $0.1 \times 250 \times 70 / 2 = 875 \text{ } \mu\text{g.L}^{-1}$.

3.3.6 Derivation of MAC_{eco}

The $\text{MAC}_{\text{eco, water}}$ can be based on the LC50 of $9 \text{ } \mu\text{g.L}^{-1}$ for *Daphnia magna*. Since LAB has no potential to bioaccumulate, an assessment factor of 100 will be applied. The initial $\text{MAC}_{\text{eco, water}}$ is: $9 / 100 = 90 \text{ ng.L}^{-1}$. This value is lower than the $\text{MPC}_{\text{eco, water}}$ of $0.75 \text{ } \mu\text{g.L}^{-1}$. 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 is the $\text{MAC}_{\text{eco, water}}$ set equal to the $\text{MPC}_{\text{eco, water}}$: $0.75 \text{ } \mu\text{g.L}^{-1}$.

The $\text{MAC}_{\text{eco, marine}}$ is set a factor 10 lower than the initial $\text{MAC}_{\text{eco, water}}$ since there are no data for additional marine taxa. The crustacea in Table 8 does not account as an additional marine taxonomic group since it has the same life form and feeding strategy as freshwater crustacea like *Daphnia* sp. The initial $\text{MAC}_{\text{eco, marine}}$ is: $90 / 10 = 9 \text{ ng.L}^{-1}$. This value is lower than the $\text{MPC}_{\text{eco, marine}}$ of $0.075 \text{ } \mu\text{g.L}^{-1}$. Therefore is the $\text{MAC}_{\text{eco, marine}}$ set equal to the $\text{MPC}_{\text{eco, marine}}$: $0.075 \text{ } \mu\text{g.L}^{-1}$. It has to be noted that this procedure for the $\text{MAC}_{\text{eco, marine}}$ is currently not agreed upon. Therefore the $\text{MAC}_{\text{eco, marine}}$ needs to be re-evaluated once an agreed procedure is available.

3.3.7 Derivation of NC

The NC_{water} and $\text{NC}_{\text{marine}}$ are set a factor 100 lower than the final MPC. The NC_{water} is: 7.5 ng.L^{-1} ; the $\text{MPC}_{\text{marine}}$ is 0.75 ng.L^{-1} .

3.3.8 Derivation of $\text{SRC}_{\text{eco, aquatic}}$

The toxicity for most species as presented in table 7 and 8 is above the water solubility. Only the species with a bounded value should be used. It should be noted that in this case the $\text{SRC}_{\text{eco, aquatic}}$ will be based on only one species, *Daphnia magna*. The only chronic value is 0.0075 mg.L^{-1} . For the acute value the geometric mean of the range given for *D. magna* divided by 10 results in a value of 0.0027 mg.L^{-1} . The SRC based on the acute data is the lowest value, therefore, the $\text{SRC}_{\text{eco, aquatic}}$ will be: 0.0027 mg.L^{-1} . The $\text{SRC}_{\text{eco, aquatic}}$ is valid for the marine and the freshwater environment.

3.4 Toxicity data and derivation of ERLs for sediment

An overview of the selected freshwater sediment toxicity data for LAB is given in Table 9.

Table 9. LAB: selected freshwater sediment data for ERL derivation.

| Chronic | | Acute | |
|---------------------------|--|---------------------------|--------------------|
| Taxonomic group | NOEC/EC10 | Taxonomic group | L(E)C50 |
| Insecta | | Insecta | |
| <i>Chironomus tentans</i> | >0.125 mg.L ⁻¹ ^a | <i>Chironomus tentans</i> | >solubility (NOEC) |

^a water spiked; initial concentration in water phase of flow-through system

3.4.1 Derivation of MPC_{sediment}

In the RAR the PNEC_{water, sediment} has been calculated using equilibrium partitioning according to the old TGD of 1996. The derived value is 0.32 mg/kg_{ww}. According to Janssen et al. (2004) PNEC_{water, sediment} values derived according to the old TGD should be converted to dry weight using a PNEC_{dry}/PNEC_{wet} ratio of 2.6 rather than 4.6. The PNEC_{water, sediment} = 0.32 x 2.6 = 0.83 mg.kg_{dwt}⁻¹. This value can be recalculated to obtain the MPC_{water, sediment} for Dutch standard sediment using the Foc_{sed, TGD} of 0.05 rather than the Foc_{susp, TGD} of 0.1. The MPC_{water, sediment} is 0.83 x 0.0588 / 0.05 = 0.97 mg.kg_{dwt}⁻¹ for Dutch standard sediment.

No marine sediment data is available to derive an MPC_{marine, sediment} for the marine environment. Therefore, the MPC_{marine, sediment} is derived from the MPC_{eco, marine} using equilibrium partitioning according to the TGD of 2003. The MPC_{marine, sediment} is 97 µg.kg_{dwt}⁻¹ for Dutch standard sediment.

3.4.2 Derivation of NC_{sediment}

The NC is set a factor 100 lower than the MPC. The NC_{sediment, water} is: 9.7 µg.kg_{dwt}⁻¹ and the NC_{marine, sediment} is 0.97 µg.kg_{dwt}⁻¹.

3.4.3 Derivation of SRC_{eco, sediment}

Not enough toxicity data is available to derive an SRC_{eco} for the sediment compartment from experimental toxicity data. Therefore, the SRC_{eco, sediment} is derived from the SRC_{eco, aquatic} using equilibrium partitioning. The SRC_{eco, sediment} is 3.5 mg.kg_{dwt}⁻¹ for Dutch standard sediment. The SRC_{eco, sediment} is valid for marine and freshwater sediment.

3.5 Toxicity data and derivation of ERLs for soil

No toxicity data on terrestrial organisms are reported in the RAR.

3.5.1 Derivation of MPC_{soil}

3.5.1.1 MPC_{eco, soil}

No toxicity data on terrestrial organisms is available, therefore, in the RAR, the PNEC_{terrestrial organisms} has been calculated from the PNEC_{aquatic organisms} using equilibrium partitioning. The derived PNEC_{terrestrial organisms} is 0.29 mg/kg for wet soil. To derive an MPC_{eco, soil} the PNEC_{terrestrial organisms} has been recalculated for dry Dutch standard soil. The MPC_{eco, soil} is: 0.97 mg.kg_{dwt}⁻¹ for Dutch standard soil.

3.5.1.2 MPC_{human, soil}

The MPC_{human, soil} is based on the TDI of 250 $\mu\text{g}\cdot\text{kg}_{\text{bw}}^{-1}\cdot\text{day}^{-1}$ with the method as described in Van Vlaardingen and Verbruggen (2007) with the mean logKow for LAB as given in Table 3. 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 2.1 $\mu\text{g}\cdot\text{kg}_{\text{dwt}}^{-1}$ for Dutch standard soil.

3.5.1.3 Selection of the MPC_{soil}

The lowest MPC_{soil} is the MPC_{human, soil}: 2.1 $\mu\text{g}\cdot\text{kg}_{\text{dwt}}^{-1}$ Dutch standard soil.

3.5.2 Derivation of NC_{soil}

The NC_{soil} is set a factor of 100 lower than the MPC_{soil}: NC_{soil} = 21 $\text{ng}\cdot\text{kg}_{\text{dwt}}^{-1}$ Dutch standard soil.

3.5.3 Derivation of SRC_{eco, soil}

No data is available on effects to terrestrial organisms that can be used for calculation of the SRC_{eco, soil}. Therefore, the SRC_{eco, soil} is derived from the SRC_{eco, water} using equilibrium partitioning. The SRC_{eco, soil} is 3.5 $\text{mg}\cdot\text{kg}_{\text{dwt}}^{-1}$ for Dutch standard soil.

3.6 Derivation of ERLs for groundwater

3.6.1 Derivation of MPC_{gw}

3.6.1.1 MPC_{eco, gw}

Since groundwater-specific exotoxicological ERLs for the groundwater compartment are absent, the surface water MPC_{eco, water} is taken as substitute. Thus, MPC_{eco, gw} = MPC_{eco, water} = 0.75 $\mu\text{g}\cdot\text{L}^{-1}$.

3.6.1.2 MPC_{human, gw}

The MPC_{human, gw} is set equal to the MPC_{dw, water}. Therefore the MPC_{human, gw} = MPC_{dw, water}: 875 $\mu\text{g}\cdot\text{L}^{-1}$.

3.6.1.3 Selection of the MPC_{gw}

The lowest MPC is the MPC_{eco, gw} of 0.75 $\mu\text{g}\cdot\text{L}^{-1}$. Thus, the final MPC_{gw} = 0.75 $\mu\text{g}\cdot\text{L}^{-1}$.

3.6.2 Derivation of NC_{gw}

The NC_{gw} is set a factor 100 lower than the MPC_{gw}. Thus, NC_{gw} = 0.75/100 = 0.0075 $\mu\text{g}\cdot\text{L}^{-1}$ = 7.5 $\text{ng}\cdot\text{L}^{-1}$

3.6.3 Derivation of SRC_{eco, gw}

The SRC_{eco, gw} is set equal to SRC_{eco, aquatic}: 0.0027 $\text{mg}\cdot\text{L}^{-1}$.

3.7 Derivation of ERLs for air

3.7.1 Derivation of MPC_{eco, air}

No ecotoxicological data for the atmospheric compartment is reported in the RAR. Therefore no MPC_{eco, air} can be derived.

3.7.2 Derivation of MPC_{human, air}

A TCA for LAB of $90 \mu\text{g}\cdot\text{m}^{-3}$ has been derived, this value will set the MPC_{human, air}. Therefore the MPC_{human, air} is $90 \mu\text{g}\cdot\text{m}^{-3}$.

3.7.3 Selection of the MPC_{air}

The only MPC_{air} available is the MPC_{human, air} this one will therefore set the MPC_{air}: $90 \mu\text{g}\cdot\text{m}^{-3}$.

3.7.4 Derivation of NC_{air}

The MPC_{air} divided by 100 is the NC_{air}: $0.9 \mu\text{g}\cdot\text{m}^{-3}$.

3.8 Comparison of derived ERLs with monitoring data

The RIWA (Dutch Association of River Water companies) does not present any monitoring data for LAB 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 LAB on their website (www.waterstat.nl). The RAR reports monitoring data from the USA for 1991. They give ranges from below the detection limit ($0.1 \mu\text{g}\cdot\text{L}^{-1}$) to $1.0 \mu\text{g}\cdot\text{L}^{-1}$ for water downstream of a sewage treatment plant. This highest value is above the MPC_{water} of $0.75 \mu\text{g}\cdot\text{L}^{-1}$ derived in this report.

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 LAB in water, groundwater, sediment, 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. Monitoring data for LAB in the Dutch environment are not available. Therefore it cannot be judged if the derived ERLs are being exceeded.

Table 10. Derived MPC, NC, MAC_{eco} , and SRC_{eco} values for LAB.

| ERL | unit | value | | | |
|-----------------------------------|-----------------------------|----------------------|----------------------|----------------------|-------------------|
| | | MPC | NC | MAC_{eco} | SRC_{eco} |
| water ^a | $\mu\text{g.L}^{-1}$ | 0.75 | 7.5×10^{-3} | 0.75 | 2.7 |
| water susp. matter. ^c | mg.kg_{dwt}^{-1} | 1.8 | | | |
| drinking water ^b | mg.L^{-1} | 0.88 | | | |
| marine | $\mu\text{g.L}^{-1}$ | 7.5×10^{-2} | 7.5×10^{-4} | 7.5×10^{-2} | 2.7 |
| marine susp. matter. ^c | mg.kg_{dwt}^{-1} | 0.19 | | | |
| water, sediment ^d | mg.kg_{dwt}^{-1} | 0.97 | 9.7×10^{-3} | | 3.5 |
| marine, sediment ^d | mg.kg_{dwt}^{-1} | 9.7×10^{-2} | 9.7×10^{-4} | | 3.5 |
| soil ^e | $\mu\text{g.kg}_{dwt}^{-1}$ | 2.1 | 2.1×10^{-2} | | 3.5×10^3 |
| groundwater | $\mu\text{g.L}^{-1}$ | 0.75 | 7.5×10^{-3} | | 2.7 |
| air | $\mu\text{g.m}^{-3}$ | 90 | 0.90 | | |

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

^b 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.

^c Expressed on the basis of Dutch standard suspended matter.

^d Expressed on the basis of Dutch standard sediment.

^e Expressed on the basis of Dutch standard soil.

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