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

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Abstract

Environmental risk limits for xylenes (m-xylene, o-xylene and p-xylene)

This report documents the RIVM derivation of environmental risk limits (ERLs) for xylenes in water, groundwater and soil. This group of substances contains m-xylene, o-xylene and p-xylene. These substances are used as solvents in the printing, rubber and leather industries.

For deriving the ERLs, RIVM used up-to-date ecotoxicological data in combination with the most recent methodology, as required by the European Water Framework Directive. This resulted in ERLs for fresh surface water that are reduced compared to earlier derived ERLs. However, monitoring data from the river Rhine in the period 2001 - 2006 do not show an exceedance of the new ERLs. ERLs were not derived for the sediment compartment, because sorption to sediment is below the trigger value to derive such risk limits, resulting in minimal exposure of water organisms to xylenes via the sediment.

ERLs are not legally binding, but provide the scientific basis for setting the Environmental Quality Standards, a task which falls under the authority of the Dutch interdepartmental 'Steering Group Substances'. The government adopts these quality standards when implementing the national policy on substances and the European Water Framework Directive. Four different risk limits are distinguished: 'Negligible Concentrations' (NC); the concentration at which no harmful effects are to be expected ('Maximum Permissible Concentration', MPC); the 'Maximum Acceptable Concentration' for ecosystems – specifically in terms of short-term exposure (MAC_{eco}); and the concentration at which possible serious effects are to be expected ('Serious Risk Concentrations', SRC_{eco}).

Key words:
environmental risk limits, negligible concentration, maximum permissible concentration, maximum acceptable concentration, serious risk concentration, xylene, 1,2-dimethylbenzene, 1,3-dimethylbenzene, 1,4-dimethylbenzene

Rapport in het kort

Milieurisicogrenzen voor xylenen (m-xyleen, o-xyleen, p-xyleen)

Het RIVM heeft milieurisicogrenzen afgeleid voor xylenen in water, grondwater en bodem. Deze stoffen worden gebruikt als oplosmiddel bij drukkerijen en in de rubberindustrie. De groep stoffen omvat m-xyleen, o-xyleen en p-xyleen.

Voor dit onderzoek zijn actuele (eco)toxicologische gegevens gebruikt, gecombineerd met de meest recente methodiek. Deze methodiek is voorgeschreven door de Europese Kaderrichtlijn Water. De nieuwe milieurisicogrenzen zijn lager dan de eerder afgeleide milieurisicogrenzen. Gemeten concentraties in de Rijn tussen 2001 en 2006 laten geen overschrijding van de nieuwe milieurisicogrenzen zien. Voor de waterbodem zijn geen milieurisicogrenzen afgeleid, omdat de xylenen de grenswaarde voor binding aan sediment niet overschrijden. Hierdoor is blootstelling van waterorganismen aan xylenen via sediment minimaal.

Milieurisicogrenzen zijn niet bindend, maar zijn de wetenschappelijke basis waarop de Nederlandse interdepartementale Stuurgroep Stoffen de wettelijke milieukwaliteitsnormen vaststelt. De overheid hanteert deze normen bij de uitvoering van het nationale stoffenbeleid en de Europese Kaderrichtlijn Water. Er bestaan vier verschillende niveaus voor milieurisicogrenzen: een Verwaarloosbaar Risiconiveau (VR), een niveau waarbij geen schadelijke effecten zijn te verwachten, het Maximaal Toelaatbaar Risiconiveau (MTR), de Maximaal Aanvaardbare Concentratie voor ecosystemen, specifiek voor kortdurende blootstelling (MAC_{eco}) en het Ernstig Risiconiveau, een niveau waarbij mogelijk ernstige effecten voor ecosystemen zijn te verwachten (ER_{eco}).

Trefwoorden:
milieurisicogrenzen, verwaarloosbaar risiconiveau, maximaal toelaatbaar risiconiveau, maximaal acceptabele concentratie, ernstig risiconiveau, xyleen, 1,2-dimethylbenzeen, 1,3-dimethylbenzeen, 1,4-dimethylbenzeen

Preface

The goal of this report is to derive risk limits that protect both man and the environment. This is done in accordance with the methodology of the Water Framework Directive (WFD) that is incorporated in the present International and National Environmental Quality Standards for Substances in the Netherlands (INS) methodology, following the Guidance for the derivation of environmental risk limits within the INS framework (Van Vlaardingen and Verbruggen, 2007).

The results presented in this report have been discussed by the members of the scientific advisory group for the project 'International and National Environmental Quality Standards for Substances in the Netherlands' (WK-INS). This advisory group provides a non-binding scientific advice on the final draft of a report in order to advise the Dutch Steering Group for Substances of the project INS on the scientific merits of the report.

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The results of the present report have been discussed in the scientific advisory group INS (WK INS). The members of this group are acknowledged for their contribution.

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Contents

Summary

Environmental risk limits are derived using ecotoxicological, physico-chemical, and human toxicological data. They represent potential risks of a substance to man and ecosystems and form the scientific basis for setting environmental quality standards by the Dutch Steering Group for Substances.

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 m-xylene, o-xylene and p-xylene in water, groundwater, soil and air. No risk limits were derived for the sediment compartment because sorption to sediment is below the trigger value to derive such risk limits.

The methodology used for the derivation of the MPC and MAC_{eco} for water, soil and air is in accordance with the Water Framework Directive. This methodology is based on the Technical Guidance Document (TGD) on risk assessment for new and existing substances and biocides (EC, 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 the river Rhine from the years 2001-2006, obtained from RIWA (Association of River Waterworks), show that at all sampling occasions and locations, the concentration of m-, o-, and p-xylene in water was below detection limits (0.02 µg/L). Based on these data, the new ERLs are not exceeded.

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

ERL	Unit	Substance	MPC	MAC	NC	SRC
Freshwater	µg/L	m-xylene	2.44	24.4	0.24	700
Marine water	µg/L	m-xylene	0.24	2.44	0.02	n.a.[b]
Soil	µg/kg	m-xylene	31.9	n.a.[b]	0.32	n.d.[a]
Groundwater	µg/L	m-xylene	2.44	n.a.[b]	0.02	n.a.[b]
Air	µg/m^3	m-xylene	870	n.a.[b]	n.a.[b]	n.a.[b]
Freshwater	µg/L	o-xylene	4.10	41.0	0.04	1000
Marine water	µg/L	o-xylene	0.41	8.2	0.004	n.a.[b]
Soil	µg/kg	o-xylene	56.0	n.a.[b]	0.56	n.d.[a]
Groundwater	µg/L	o-xylene	4.10	n.a.[b]	0.04	n.a.[b]
Air	µg/m^3	o-xylene	870	n.a.[b]	n.a.[b]	n.a.[b]
Freshwater	µg/L	p-xylene	2.60	26.0	0.03	749
Marine water	µg/L	p-xylene	0.26	2.60	0.003	n.a.[b]
Soil	µg/kg	p-xylene	37.2	n.a.[b]	0.37	n.d.[a]
Ground water	µg/L	p-xylene	2.60	n.a.[b]	0.03	n.a.[b]
Air	µg/m^3	p-xylene	870	n.a.[b]	n.a.[b]	n.a.[b]
Freshwater	µg/L	xylene	2.44	24.4	0.02	922
Marine water	µg/L	xylene	0.24	4.88	0.002	n.a.[b]
Soil	µg/kg	xylene	33.35	n.a.[b]	0.33	n.d.[a]
Ground water	µg/L	xylene	2.44	n.a.[b]	0.02	n.a.[b]
Air	µg/m^3	xylene	870	n.a.[b]	n.a.[b]	n.a.[b]

[a] n.d. = not derived due to lack of data

[b] n.a. = not applicable

1 Introduction

1.1 Project framework

In this report, environmental risk limits (ERLs) for surface water (freshwater and marine) are derived for m-xylene, o-xylene and p-xylene. 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 below) 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} death per year can be calculated (for carcinogenic substances).
- Maximum Acceptable Concentration (MAC_{eco}) – concentration protecting aquatic ecosystems for effects due to short-term exposure or concentration peaks.
- Serious Risk Cconcentration (SRC_{eco}) – concentration at which possibly serious ecotoxicological effects are to be expected.

These ERLs serve as advisory values that are used by the Steering Group for Substances to set Environmental Quality Standards (EQS) for various policy purposes. EQSs are all legally and non legally binding standards that are used in Dutch environmental policy.

1.2 Selection of substances

ERLs are derived for m-xylene, o-xylene and p-xylene (Table 2), which were selected by the Netherlands within the framework of ‘International and national environmental quality standards for substances in the Netherlands’ (INS).

Table 2. Selected compounds.

Compound	CAS number
m-xylene	108-38-3
o-xylene	95-47-6
p-xylene	106-42-3

1.3 Guidance followed for this project

In this report ERLs are derived following the methodology of the project ‘International and national environmental quality standards for substances in the Netherlands’ (INS) (Van Vlaardingen and Verbruggen, 2007). This updated INS guidance is in accordance with the guidance by Lepper (2005) which forms part of the Priority Substances Daughter Directive (2006/0129 (COD)) amending the WFD (2000/60/EC). The WFD guidance applies to the derivation of MPCs for water and sediment. ERL derivations for water and sediment are performed for both the freshwater and marine compartment. The WFD guidance introduces a new ERL, which is the Maximum Acceptable Concentration (MAC_{eco}), a concentration that protects aquatic ecosystems from adverse effects caused by short-term exposure or concentration peaks. Two MPC values are considered for the water compartment that are based on a human toxicological risk limit (TL_{hh}), such as an ADI or TDI (Acceptable or Tolerable Daily Intake, respectively). Discerned are (1) the $MPC_{hh\ food,\ water}$, which is the concentration in water that should protect humans against adverse effects from the substance via fish and shellfish consumption; (2) the $MPC_{dw,water}$, which is the concentration in water that should protect humans against adverse effects of the substance by consumption of drinking water. Note that each of these two MPCs is allowed to contribute only 10% to the TL_{hh}. Two other MPCs are derived for the water compartment, based on ecotoxicological data. These are (1) the $MPC_{eco,water}$, which is based on direct aquatic ecotoxicological data and (2) the $MPC_{sp,water}$, the MPC accounting for secondary poisoning, which is derived in case secondary poisoning in the environment is thought to be of concern. It is important to note that MPC derivation integrates both ecotoxicological data and a human toxicological threshold value. The value of this final ‘environmental risk limit’ is determined by the lowest of these protection objectives.

The WFD guidance departs from the viewpoint that laboratory toxicity tests contain suspended matter in such concentrations, that results based on laboratory tests are comparable to outdoor surface waters. In other words: each outcome of an ERL derivation for water will now result in a total concentration. A recalculation from a dissolved to a total concentration is thus no longer made within INS framework. This differs from the former Dutch approach, in which each outcome of a laboratory test was considered to represent a dissolved concentration. This concentration could then be recalculated to a total concentration using standard characteristics for surface water and suspended matter.

2 Methods

The methodology for the derivation of ERLs is described in detail by Van Vlaardingen and Verbruggen (2007), further referred to as the ‘INS-Guidance’. This guidance is in accordance with the guidance of the Fraunhofer Institute (FHI; Lepper, 2005), which forms part of the Priority Substances Daughter Directive (2006/0129 (COD)) amending the WFD (2000/60/EC).

The process of ERL derivation consists of the following steps: data collection, data evaluation and selection, and derivation of the ERLs on the basis of the selected data.

2.1 Data collection

An online literature search was performed on TOXLINE (literature from 1985 to 2001) and Current contents (literature from 1997 to 2007). The search resulted in approximately 110 references, of which more than 60 references were considered relevant. In additon to this, all references in the RIVM e-tox base and EPA's ECOTOX database were evaluated (an additional 30 references). All toxicity data are reported in the Appendices.

2.2 Data evaluation and selection

Ecotoxicity studies (including bird and mammal studies) were screened for relevant endpoints (i.e. those endpoints that have consequences at the population level of the test species). All relevant ecotoxicity and bioaccumulation tests were then thoroughly evaluated with respect to the validity (scientific reliability) of the study. A detailed description of the evaluation procedure is given in the INS-Guidance (see section 2.2.2 and 2.3.2). In short, the following reliability indices (Ri) were assigned:

- Ri 1: Reliable without restriction
  ‘Studies or data … generated according to generally valid and/or internationally accepted testing guidelines (preferably performed according to GLP) or in which the test parameters documented are based on a specific (national) testing guideline … or in which all parameters described are closely related/comparable to a guideline method.’
- Ri 2: Reliable with restrictions
  ‘Studies or data … (mostly not performed according to GLP), in which the test parameters documented do not totally comply with the specific testing guideline, but are sufficient to accept the data or in which investigations are described which cannot be subsumed under a testing guideline, but which are nevertheless well documented and scientifically acceptable.’
- Ri 3: Not reliable
  ‘Studies or data … in which there are interferences between the measuring system and the test substance or in which organisms/test systems were used which are not relevant in relation to the exposure (e.g., unphysiologic pathways of application) or which were carried out or generated according to a method which is not acceptable, the documentation of which is not sufficient for an assessment and which is not convincing for an expert judgment.’

- Ri 4: Not assignable
  ‘Studies or data … which do not give sufficient experimental details and which are only listed in short abstracts or secondary literature (books, reviews, etc.).’

All available studies were summarised in data-tables, that are included as Appendices to this report. These tables contain information on species characteristics, test conditions and endpoints. Explanatory notes are included with respect to the assignment of the reliability indices.

For the xylene isomers, fast volatilisation put special demands on the way toxicity tests are performed. This implies that in some cases endpoints were not considered reliable, although the test was performed and documented according to accepted guidelines. When xylene concentrations were not monitored in an open test system, a Ri of 3 was attributed to the study.

Endpoints with Ri 1 or 2 are accepted as valid, but this does not automatically mean that the endpoint is selected for the derivation of ERLs. The validity scores are assigned on the basis of scientific reliability, but valid endpoints may not be relevant for the purpose of ERL-derivation (e.g. due to inappropriate exposure times or test conditions that are not relevant for the Dutch situation).

After data collection and validation, toxicity data were combined into an aggregated data table with one effect value per species according to section 2.2.6 of the INS-Guidance. When for a species several effect data were available, the geometric mean of multiple values for the same endpoint was calculated where possible. Subsequently, when several endpoints were available for one species, the lowest of these endpoints (per species) is reported in the aggregated data table.

2.3 Derivation of ERLs

For a detailed description of the procedure for derivation of the ERLs, reference is made to the INS-Guidance. For some parts of the present ERL-derivation, however, additional comments should be made.

2.3.1 Drinking water

In the FHI Guidance, Lepper (2005) states that the lowest MPC value should be selected as the general MPC. In line with this, 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 for the general MPC_{water} (see INS-Guidance, section 3.1.6 and 3.1.7). In the proposal for the daughter directive Priority Substances, however, the EC based the derivation of the AA-EQS (= MPC) 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 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 Waterkwaliteitseisen 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.

Related to this is the inclusion of water treatment for the derivation of the $MPC_{dw, water}$. According to the INS-Guidance, a substance specific removal efficiency related to simple water treatment should be derived.

2.3.2 $MAC_{eco,\ marine}$

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 derived 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

3.1 m-xylene

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

3.1.1.1 Identity

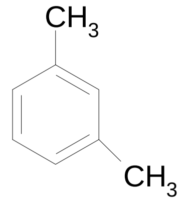

Figure 1. Structural formula of m-xylene.

Table 3. Identification of m-xylene.

Parameter	Name or number	Source
Chemical name	1,3-dimethylbenzene	Mackay et al., 2006
Common/trivial/other name	meta-xylene, m-xylol, 3-methyltoluene	Mackay et al., 2006
CAS number	108-38-3	Mackay et al., 2006
EC number	203-576-3	
SMILES code	Cc1cccc(C)c1	

3.1.1.2 Physico-chemical properties

Table 4. Physico-chemical properties of m-xylene.

Parameter	Unit	Value	Remark	Reference
Molecular weight	[g/mol]	106.165		Mackay et al., 2006
Water solubility	[mg/L]	160	25°C	Mackay et al., 2006
log K_{OW}	[-]	3.15		Mackay et al., 2006
log K_{OC}	[-]	2.33	OC ≥ 0.5%	Mackay et al., 2006
Vapour pressure	[Pa]	833	20°C	Mackay et al., 2006
		1213	30°C	
		6400	59.3°C	
Melting point	[°C]	-47.8		Mackay et al., 2006
Boiling point	[°C]	139.12		Mackay et al., 2006
Henry's law constant	[Pa.m^3/mol]	615	EPIC-GC-FID, 2-25°C	Mackay et al., 2006

3.1.1.3 Behaviour in the environment

Table 5. Selected environmental properties of m-xylene.

Parameter	Unit	Value	Remark	Reference
Hydrolysis half-life	DT50 [d]		no hydrolysable functional groups	Mackay et al., 2006
Photolysis half-life	DT50 [d]	0.4		IUCLID, 2000

In water, volatilisation seems to be the dominant removal process (Mackay et al., 2006) with a half-life of 3.1 hours (depth 1m, wind speed 3 m/s, current 1m/s).

3.1.1.4 Bioconcentration and biomagnification

An overview of the bioaccumulation data for m-xylene is given in Table 6. Detailed bioaccumulation data for m-xylene are tabulated in Appendix 1.

Table 6. Overview of bioaccumulation data for m-xylene.

Parameter	Unit	Value	Remark	Reference
BCF (molluscs)	[L/kg]	6.43		Nunes and Benville, 1979
BCF (fish)	[L/kg]	23	Exposure in crude oil suspension	Mackay et al., 2006; Ogata and Miyake, 1978
BMF	[kg/kg]	1	Default value for BCF < 2000 L/kg	Van Vlaardingen and Verbruggen, 2007

3.1.1.5 Human toxicological threshold limits and carcinogenicity

The following R-phrases are assigned to m-xylene: R10, R20/21, R38; m-xylene is not classified as being a carcinogen. The Tolerable Daily Intake (TDI) for xylenes is 150 μg/kg bw day (Baars et al., 2001).

3.1.2 Trigger values

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

Table 7. m-xylene: collected properties for comparison to ERL triggers.

Parameter	Value	Unit	Method/Source	Derived at section
Log $K_{p,\mathrm{susp\text{-}water}}$	1.33	[-]	$K_{OC} \times f_{OC,\mathrm{susp}}$[1]	K_{OC}: 3.1.1.2
BCF	23	[L/kg]		3.1.1.4
BMF	1	[kg/kg]		3.1.1.4
Log K_{OW}	3.15	[-]		3.1.1.2
R-phrases	R10, R20/21, R38	[-]		3.1.1.5
A1 value	not available	[μg/L]		
DW standard	not available	[μg/L]		

1 $f_{OC,\mathrm{susp}} = 0.1\ \mathrm{kg_{OC}/kg_{solid}}$ (EC, 2003).

- m-xylene has a log $K_{\mathrm{p, susp\text{-}water}} < 3$; derivation of $\mathrm{MPC}_{\mathrm{sediment}}$ is not triggered.
- m-xylene has a log $K_{\mathrm{p, susp\text{-}water}} < 3$; expression of the $\mathrm{MPC}_{\mathrm{water}}$ as $\mathrm{MPC}_{\mathrm{susp, water}}$ is not required.
- m-xylene has a BCF < 100 L/kg; assessment of secondary poisoning is not triggered.
- For m-xylene, no A1 and no Drinking Water value are available from Council Directives 75/440, EEC and 98/83/EC, respectively. Therefore, a provisional Drinking Water Standard (DWS) needs to be derived.

3.1.3 Toxicity data and derivation of ERLs for water

3.1.3.1 $\mathrm{MPC}_{\mathrm{eco, water}}$ and $\mathrm{MPC}_{\mathrm{eco, marine}}$

An overview of the selected toxicity data for m-xylene is given in Table 8 (freshwater) and Table 9 (marine water). Detailed toxicity data for m-xylene are tabulated in Appendix 2.

Table 8. m-xylene: selected freshwater toxicity data for ERL derivation.

Chronic[a] **Taxonomic group**	**NOEC/EC10 (mg/L)**	**Acute**[a] **Taxonomic group**	**L(E)C50 (mg/L)**
Algae		Algae	
Pseudokirchneriella subcapitata	0.7	*Scenedesmus quadricauda*	7.43
		Crustacea	
		Cerodaphnia cf. dubia	**2.44**
		Daphnia magna	10.57[b]
		Daphnia spinulata	4.25
		Hyalella curvispina	4.25
		Pisces	
		Bryconamericus iheringii	11.45[c]
		Carassius auratus	10.72
		Oncorhynchus mykiss	8.40
		Oryzias latipes	32.00
		Pimephales promelas	15.49
		Poecilia reticulata	12.90

[a] For detailed information see Appendix 2. Bold values are used for ERL derivation.
[b] Geometric mean of 4.70 and 23.77 mg/L; parameter immobility.
[c] Geometric mean of 11.68 and 11.23 mg/L.

Table 9. m-xylene: selected marine toxicity data for ERL derivation.

Chronic [a] **Taxonomic group**	**NOEC/EC10 (mg/L)**	**Acute** [a] **Taxonomic group**	**L(E)C50 (mg/L)**
		Bacteria	
		Vibrio fischeri	19.31
		Crustacea	
		Artemia salina	10.80

[a] For detailed information see Appendix 2.

3.1.3.2 Treatment of fresh- and saltwater toxicity data

The datasets were compared according to the guidance of Van Vlaardingen and Verbruggen (2007). Based on the result of the t-test ($\alpha > 0.05$), the fresh- and saltwater data can be combined.

3.1.3.3 Mesocosm studies

No mesocosm studies were available for m-xylene.

3.1.3.4 Derivation of $MPC_{eco, water}$ and $MPC_{eco, marine}$

Freshwater

The base set is complete. However, since only one chronic NOEC for algae (0.7 mg/L) is available an assessment factor of 1000 should be used on the lowest $L(E)C_{50}$ value. In this case, the lowest $L(E)C_{50}$ value is 2.44 mg/L for *Cerodaphnia cf. dubia*, resulting in a $MPC_{eco, water}$ of 2.44 mg/L / 1000 = 2.44 µg/L

Marine water

Since the datasets for freshwater and marine water can be combined, the $MPC_{eco, marine}$ is derived by applying an assessment factor of 10000 on the EC_{50} value of 2.44 mg/L for *Cerodaphnia cf. dubia.* The $MPC_{eco, marine}$ is 2.44 mg/L / 10000 = 0.24 µg/L.

3.1.3.5 $MPC_{sp, water}$ and $MPC_{sp, marine}$

m-xylene has a BCF<100 L/kg, thus assessment of secondary poisoning is not triggered.

3.1.3.6 $MPC_{hh food, water}$

Derivation of $MPC_{hh food, water}$ for m-xylene is not triggered (Table 7).

3.1.3.7 $MPC_{dw, water}$

For m-xylene, no A1 and no Drinking Water Standard were available from Council Directives 75/440, EEC and 98/83/EC, respectively. Therefore, a provisional DWS based on the TDI value for xylenes (150 $\mu g/kg_{bw}$ day Baars et al., 2001) should be derived, using the following formula given in Van Vlaardingen and Verbruggen 2007, section 3.1.6. Using a TDI value of 150 $\mu g/kg_{bw}$ day, an average bodyweigth of 70 kg and an averaged drinking water uptake of 2L/day, the $MPC_{dw, water, provisional}$ becomes 525 µg/L.

3.1.3.8 $MPC_{human, water}$

Following WFD methodology, the derivation of the $MPC_{human, water}$ is integrated in the MPC derivation for the water compartment. Since derivation of $MPC_{hh food, water}$ for m-xylene is not triggered (Table 7), the $MPC_{human, gw}$ is equal to the $MPC_{dw, water}$ of 525 µg/L (Van Vlaardingen and Verbruggen, 2007).

3.1.4 Selection of the MPC$_{\text{water}}$ and MPC$_{\text{marine}}$

Freshwater

The lowest MPC value of the routes included is the MPC$_{\text{eco,water}}$ (see section 2.3). Therefore, the MPC$_{\text{water}}$ is 2.44 µg/L.

Marine water

The lowest value of the routes included is the MPC$_{\text{eco, marine}}$ (see section 2.3). Therefore, the MPC$_{\text{marine}}$ is 0.24 µg/L.

3.1.4.1 MAC$_{\text{eco, water}}$

Since the base set for m-xylene is complete, the substance does not bioaccumulate (BCF < 100 L/kg), and the mode of toxic action is known (nonpolar narcosis), an assessment factor of 100 can be used for the derivation of the MAC$_{\text{eco, water}}$. Based on the lowest EC$_{50}$ value of 2.44 mg/L for *Cerodaphnia cf. dubia*, this results in a MAC$_{\text{eco, water}}$ of 2.44mg/L / 100 = 24.4 µg/L.

3.1.4.2 MAC$_{\text{eco, marine}}$

Since the datasets for freshwater and marine water can be combined and no data on the toxicity of m-xylene for specific marine taxonomic groups is available, the MAC$_{\text{eco, marine}}$ is derived by applying an additional assessment factor of 10 on the MAC$_{\text{eco, water}}$ of 24.4 µg/L.
The MAC$_{\text{eco, marine}}$ is 24.4 µg/L / 10 = 2.44 µg/L.

3.1.4.3 NC$_{\text{water}}$

According to Van Vlaardingen en Verbruggen (2007), the NC should be *'set to a factor of 100 below the MPC, which defines a safety margin allowing for combination toxicity.'* Thus, the NC$_{\text{water}}$ for m-xylene is the MPC$_{\text{water}}$ of 2.44 µg/L / 100 = 0.24 µg/L.

3.1.4.4 NC$_{\text{marine}}$

According to Van Vlaardingen en Verbruggen (2007), the NC should be *'set to a factor of 100 below the MPC, which defines a safety margin allowing for combination toxicity.'* Thus, the NC$_{\text{marine}}$ for m-xylene is the MPC$_{\text{marine}}$ of 0.24 µg/L / 100 = 0.02 µg/L.

3.1.4.5 SRC$_{\text{eco, water}}$

The base set is complete and one NOEC for algae (0.7 mg/L) is available. The datasets for freshwater and marine water were combined, the geometric mean of the combined L(E)C$_{50}$ values is 9.44 mg/L. Since this geometric mean is more than 10 times higher than the NOEC, the SRC$_{\text{eco, water}}$ is based on the NOEC using an assessment factor of 1 (Van Vlaardingen and Verbruggen, 2007).
The SRC$_{\text{eco, water}}$ for m-xylene is 0.7 mg/L = 700 µg/L.

3.1.5 Toxicity data and derivation of ERLs for sediment

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

3.1.6 Toxicity data and derivation of ERLs for soil

3.1.6.1 MPC$_{\text{eco, soil}}$

Since soil data for m-xylene are not available, the equilibrium partitioning method was used (Van Vlaardingen and Verbruggen, 2007, section 3.7). Using $K_{\text{air-water}}$ = 0.26 m^3/m^3, Kp_{soil} = 4.3 L/kg, $K_{\text{soil-water}}$ = 6.67, the $MPC_{\text{Dutch standard soil, EqP, dwt}}$ is calculated to be 31.9 µg/kg.

3.1.6.2 MPC$_{\text{sp, soil}}$

m-xylene has a BCF<100 L/kg, thus assessment of secondary poisoning is not triggered.

3.1.6.3 MPC$_{\text{human, soil}}$

According to the methods in the INS Guidance (Van Vlaardingen and Verbruggen, 2007, section 3.3.6), the $MPC_{\text{human,soil, dwt}}$ is 1.693 mg/kg = 1693 µg/kg for consumption of root crops.

3.1.6.4 MPC$_{\text{soil}}$

The lowest value of the routes included is the $MPC_{\text{eco, soil}}$ (see section 2.3). Therefore, the MPC_{soil} is 31.9 µg/L.

3.1.6.5 NC$_{\text{soil}}$

According to Van Vlaardingen en Verbruggen (2007), the NC should be *'set to a factor of 100 below the MPC, which defines a safety margin allowing for combination toxicity.'* Thus, the NC_{soil} for m-xylene is the MPC_{soil} of 31.9 µg/kg / 100 = 0.32 µg/kg.

3.1.6.6 SRC$_{\text{soil}}$

Since no toxicity data are available, the SRC_{soil} can not be derived.

3.1.7 Derivation of ERLs for groundwater

Since groundwater-specific ecotoxicological data are not available for m-xylene, the ERLs for surface water and drinking water are taken as substitute (Van Vlaardingen and Verbruggen, 2007).

3.1.7.1 MPC$_{\text{eco, gw}}$

The $MPC_{\text{eco, gw}}$ is equal to the $MPC_{\text{eco, water}}$ of 2.44 µg/L.

3.1.7.2 MPC$_{\text{human, gw}}$

The $MPC_{\text{human, gw}}$ is equal to the $MPC_{\text{dw, water}}$ of 525 µg/L.

3.1.7.3 MPC$_{\text{gw}}$

The lowest value of the routes included is the $MPC_{\text{eco, gw}}$ (see section 2.3). Therefore, the MPC_{gw} is 2.44 µg/L.

3.1.7.4 NC$_{\text{gw}}$

According to Van Vlaardingen en Verbruggen (2007), the NC should be *'set to a factor of 100 below the MPC, which defines a safety margin allowing for combination toxicity.'* Thus, the NC_{gw} for m-xylene is the MPC_{gw} of 2.44 µg/L / 100 = 0.02 µg/L.

3.1.8 Derivation of ERL for air

3.1.8.1 $MPC_{human,\ air}$

According to Van Vlaardingen and Verbruggen (2007): '*Human exposure via air is covered via the Tolerable Concentration in Air (TCA). The TCA is an existing standard (μg/m^3) aimed at the protection of humans from deleterious effects after continuous lifetime exposure via air.'*
In 2001, a TCA of 870 μg/m^3 was derived (Baars et al., 2001). Thus, the $MPC_{human,\ air}$ is 870 μg/m^3.

3.1.9 Comparison of derived ERLs with monitoring data

An overview of the derived ERLs is given in Table 10.

Table 10. Derived MPC, NC, MAC_{eco}, and SRC_{eco} values for m-xylene.

ERL	Unit	MPC	MAC_{eco}	NC	SRC
Freshwater[a]	μg/L	2.44	24.4	0.24	700
Marine water	μg/L	0.24	2.44	0.02	n.a.[b]
Soil	μg/kg	31.9	n.a.[b]	0.32	n.d.[a]
Groundwater	μg/L	2.44	n.a.[b]	0.02	n.a.[b]
Air	μg/m^3	870	n.a.[b]	n.a.[b]	n.a.[b]

[a] n.d. = not derived.

[b] n.a. = not applicable.

Monitoring data for the Rhine from the years 2001-2006, obtained from RIWA (Association of River Waterworks), show that at all sampling occasions and locations, the concentration of m-xylene in water was below detection limits (0.02 μg/L).

3.2 o-xylene

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

3.2.1.1 Identity

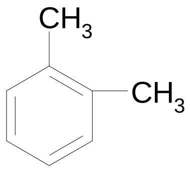

Figure 2. Structural formula of o-xylene.

Table 11. Identification of o-xylene.

Parameter	Name or number	Source
Chemical name	1,2-dimethylbenzene	Mackay et al., 2006
Common/trivial/other name	ortho-xylene, o-xylol, 2-methyltoluene	Mackay et al., 2006
CAS number	95-47-6	Mackay et al., 2006
EC number	202-422-2	
SMILES code	Cc1ccccc1C	

3.2.1.2 Physico-chemical properties

Table 12. Physico-chemical properties of o-xylene.

Parameter	Unit	Value	Remark	Reference
Molecular weight	[g/mol]	106.165		Mackay et al., 2006
Water solubility	[mg/L]	240	20°C, shake flask	Mackay et al., 2006
log K_{OW}	[-]	3.12		Mackay et al., 2006
log K_{OC}	[-]	2.35	OC $\geq$ 4.02%, Batch-equil. GC	Mackay et al., 2006
Vapour pressure	[Pa]	767 987 6354	20°C 30°C 63.5°C	Mackay et al., 2006
Melting point	[°C]	-25.2		Mackay et al., 2006
Boiling point	[°C]	144.5		Mackay et al., 2006
Henry's law constant	[Pa.m^3/mol]	594	20°C, EPICS-GC	Mackay et al., 2006

n.a. = not applicable.

3.2.1.3 Behaviour in the environment

Table 13. Selected environmental properties of o-xylene.

Parameter	Unit	Value	Remark	Reference
Hydrolysis half-life	DT50 [d]		no hydrolysable functional groups	Mackay et al., 2006
Photolysis half-life	DT50 [h]	30	27°C	IUCLID, 2000

In water, volatilisation seems to be the dominant removal process with a half-life of 3.2 hours (depth 1m, wind speed 3 m/s, current 1 m/s) (Mackay et al., 2006).

3.2.1.4 Bioconcentration and biomagnification

An overview of the bioaccumulation data for o-xylene is given in Table 14. Detailed bioaccumulation data for o-xylene are tabulated in Appendix 1.

Table 14. Overview of bioaccumulation data for o-xylene.

Parameter	Unit	Value	Remark	Reference
BCF (molluscs)	[L/kg]	7.25		Nunes and Benville, 1979
BCF (fish)	[L/kg]	21.4	Exposure in crude oil suspension	Ogata and Miyake, 1978
BMF	[kg/kg]	1	Default value for BCF < 100 L/kg	

3.2.1.5 Human toxicological threshold limits and carcinogenicity

The following R-phrases were assigned to o-xylene: R10, R20/21, R38, o-xylene is not classified as being a carcinogen. The Tolerable Daily Intake (TDI) for xylenes is 150 µg/kg bw day (Baars et al., 2001).

3.2.2 Trigger values

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

Table 15. o-xylene: collected properties for comparison to MPC triggers.

Parameter	Value	Unit	Method/Source	Derived at section
Log $K_{\mathrm{p,susp\text{-}water}}$	1.35	[-]	$K_{\mathrm{OC}} \times f_{\mathrm{OC,susp}}$[1]	K_{OC}: 3.1.1.2
BCF	21.4	[L/kg]		3.1.1.4
BMF	1	[kg/kg]		3.1.1.4
Log K_{OW}	3.12	[-]		3.1.1.2
R-phrases	R10, R20/21, R38	[-]		3.1.1.5
A1 value	not available	[µg/L]		
DW standard	not available	[µg/L]		

[1] $f_{\mathrm{OC,susp}} = 0.1\ \mathrm{kg_{OC}/kg_{solid}}$ (EC, 2003).

- o-xylene has a log $K_{\mathrm{p, susp, water}} < 3$; derivation of $\mathrm{MPC}_{\mathrm{sediment}}$ is not triggered.
- o-xylene has a log $K_{\mathrm{p, susp, water}}$, < 3; expression of the $\mathrm{MPC}_{\mathrm{water}}$ as $\mathrm{MPC}_{\mathrm{susp, water}}$ is not required.
- o-xylene has a BCF < 100 L/kg; assessment of secondary poisoning is not triggered.
- For o-xylene, 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.

3.2.3 Toxicity data and derivation of ERLs for water

3.2.3.1 $\mathrm{MPC}_{\mathrm{water, eco}}$ and $\mathrm{MPC}_{\mathrm{marine, eco}}$

An overview of the selected toxicity data for o-xylene is given in Table 16 (freshwater) and Table 17 (marine water). Detailed toxicity data for o-xylene are tabulated in Appendix 2.

Table 16. O-xylene: selected freshwater toxicity data for ERL derivation.

Chronic[a] **Taxonomic group**	**NOEC/EC10 (mg/L)**	**Acute**[a] **Taxonomic group**	**L(E)C50 (mg/L)**
Algae		Algae	
Pseudokirchnella subcapitata	1.00	*Pseudokirchneriella subcapitata*	4.70
		Scenedesmus quadricauda	27.60
		Crustacea	
		Daphnia magna	4.15[b]
		Daphnia spinulata	6.37
		Hyalella curvispina	6.37
		Pisces	
		Bryconamericus iheringii	9.75[c]
		Carassius auratus	16.10
		Catostomus commersoni	16.10
		Cnesterodon decemmaculatus	9.33
		Lepomis macrohirus	16.10
		Oncorhynchus mykiss	7.82[d]
		Pimephales promelas	16.16[e]
		Poecilia reticulata	12.00

[a] For detailed information see Appendix 2. Bold values are used for ERL derivation.

[b] Geometric mean of 1.00 and 17.22 mg/L; parameter immobilisation.

[c] Geometric mean of 9.56 and 9.94 mg/L.

[d] Geometric mean of 7.60 and 8.05 mg/L.

[e] Geometric mean of 16.10, 16.22 mg/L.

Table 17. O-xylene: selected aquatic marine data for ERL derivation.

Chronic [a]		Acute [a]	
Taxonomic group	NOEC/EC10 (mg/L)	Taxonomic group	L(E)C50 (mg/L)
		Bacteria	
		Vibrio fischeri	9.04[b]
		Crustacea	
		Artemia salina	24.64
		Echinodermata	
		Strongylocentrotus droebachiensis	**4.10**

[a] For detailed information see Appendix 2. Bold values are used for ERL derivation.
[b] Geometric mean of 9.25 and 8.83 mg/L.

3.2.3.2 Treatment of fresh- and saltwater toxicity data

The datasets were compared according to the guidance of Van Vlaardingen and Verbruggen (2007). Based on the result of the t-test ($\alpha > 0.05$), the fresh- and saltwater data can be combined.

3.2.3.3 Mesocosm studies

No mesocosm studies are available for o-xylene.

3.2.3.4 Derivation of $\text{MPC}_{\text{eco, water}}$ and $\text{MPC}_{\text{eco, marine}}$

Freshwater

The base set is complete. However, since only one chronic NOEC for algae (1 mg/L) was available an assessment factor of 1000 on the lowest L(E)C_{50} should be used, in this case 4.10 mg/L for *Strongylocnetrotus droebachiensis*, resulting in a $\text{MPC}_{\text{eco, water}}$ of 4.10 mg/L / 1000 = 4.10 µg/L.

Marine water

Since the datasets for freshwater and marine water can be combined, the $\text{MPC}_{\text{eco, marine}}$ is based on the lowest L(E)C_{50} value for *Strongylocentrotus droebachiensis* of 4.10 mg/L. Thus the $\text{MPC}_{\text{eco, marine}}$ is 4.10 mg/L / 10000 = 0.41 µg/L

3.2.3.5 $\text{MPC}_{\text{sp, water}}$ and $\text{MPC}_{\text{sp, marine}}$

o-xylene has a BCF<100 L/kg, thus assessment of secondary poisoning is not triggered.

3.2.3.6 $\text{MPC}_{\text{hh food, water}}$

Derivation of $\text{MPC}_{\text{hh food, water}}$ for o-xylene is not triggered (Table 15).

3.2.3.7 $\text{MPC}_{\text{dw, water}}$

For o-xylene, no A1 and no Drinking Water Standard are available from Council Directives 75/440, EEC and 98/83/EC, respectively. Therefore, a provisional DWS based on the TDI value for xylenes (150 µg/kg_{bw} day Baars et al., 2001) should be derived, resulting in a $\text{MPC}_{\text{dw, water}}$ of 525 µg/L (Van Vlaardingen and Verbruggen 2007, section 3.1.6).

3.2.3.8 $\text{MPC}_{\text{human, water}}$

Following WFD methodology, the derivation of the $\text{MPC}_{\text{human, water}}$ is integrated in the MPC derivation for the water compartment. Since derivation of the $\text{MPC}_{\text{hh food, water}}$ for o-xylene is not triggered (Table 15), the $\text{MPC}_{\text{human, gw}}$ is equal to the $\text{MPC}_{\text{dw, water}}$ of 525 µg/L (Van Vlaardingen and Verbruggen, 2007). Thus, the $\text{MPC}_{\text{human, water}}$ is 525 µg/L.

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

Freshwater

The lowest value of the routes included is the $MPC_{eco,water}$ (see section 2.3). Therefore, the MPC_{water} is 4.10 μg/L.

Marine water

The lowest value of the routes included is the $MPC_{eco,marine}$ (see section 2.3). Therefore, the MPC_{marine} is 0.41 μg/L.

3.2.3.10 $MAC_{eco, water}$

Since the base set for o-xylene is complete, the substance does not bioaccumulate (BCF < 100 L/kg) and the mode of toxic action is known (nonpolar narcosis), an assessment factor of 100 can be used for the derivation of the $MAC_{eco, water}$. The lowest LC_{50} value of 4.10 mg/L for *Strongylocnetrotus droebachiensis* results in a $MAC_{eco,water}$ of 4.10 mg/L / 100 = 41.0 μg/L.

3.2.3.11 $MAC_{eco, marine}$

Since the datasets for freshwater and marine water can be combined, the $MAC_{eco,marine}$ is derived by applying an additional assessment factor on the $MAC_{eco,water}$. In this case, the additional factor of 5 can be used because a value from a specific marine taxon (*Strongylocnetrotus droebachiensis*, echinodermata) is available. Therefore, the $MAC_{eco,marine}$ is 41.0 μg/L / 5 = 8.20 μg/L.

3.2.3.12 NC_{water}

According to Van Vlaardingen en Verbruggen (2007), the NC should be *'set to a factor of 100 below the MPC, which defines a safety margin allowing for combination toxicity.'* Thus, the NC_{water} for o-xylene is the MPC_{water} of 4.10 μg/L / 100 = 0.04 μg/L.

3.2.3.13 NC_{marine}

According to Van Vlaardingen en Verbruggen (2007), the NC should be *'set to a factor of 100 below the MPC, which defines a safety margin allowing for combination toxicity.'* Thus, the NC_{marine} for o-xylene is the MPC_{marine} of 0.41 μg/L / 100 = 0.004 μg/L.

3.2.3.14 SRC_{eco}

The base set is complete and one NOEC for algae (1 mg/L) is available. The datasets for freshwater and marine water were combined. The geometric mean of the combined LC_{50} values is 10.09 mg/L. Since this geometric mean is higher than 10 times the NOEC, the SRC_{eco} is based on the NOEC using an assessment factor of 1. Thus the SRC_{eco} is 1 mg/L = 1000 μg/L.

3.2.4 Toxicity data and derivation of ERLs for sediment

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

3.2.5 Toxicity data and derivation of ERLs for soil

3.2.5.1 $MPC_{eco, soil}$

Since no soil data for o-xylene were available, the equilibrium partitioning method is used (Van Vlaardingen and Verbruggen, 2007, section 3.7). Using $K_{air\text{-}water} = 0.25\ m^3/m^3$, $Kp_{soil} = 4.5$ L/kg, $K_{soil\text{-}water} = 6.97$, the $MPC_{Dutch\ standard\ soil,\ EqP,\ dwt}$ is calculated to be 56.0 μg/kg.

3.2.5.2 MPC$_{sp, soil}$

o-xylene has a BCF < 100 L/kg, thus assessment of secondary poisoning is not triggered.

3.2.5.3 MPC$_{human, soil}$

According to the methods in the INS Guidance (Van Vlaardingen and Verbruggen, 2007), the MPC$_{human, soil, dwt}$ is 1.890 mg/kg = 1890 µg/kg for consumption of root crops.

3.2.5.4 MPC$_{soil}$

The lowest value of the routes included is the MPC$_{eco, soil}$ (see section 2.3). Therefore, the MPC$_{soil}$ is 56.0 µg/L.

3.2.5.5 NC$_{soil}$

According to Van Vlaardingen en Verbruggen (2007), the NC should be *'set to a factor of 100 below the MPC, which defines a safety margin allowing for combination toxicity.'* Thus, the NC$_{soil}$ for o-xylene is the MPC$_{soil}$ of 56.0 µg/kg / 100 = 0.56 µg/kg.

3.2.5.6 SRC$_{soil}$

Since no toxicity data are available, the SRC$_{soil}$ can not be derived.

3.2.6 Derivation of ERLs for groundwater

Since groundwater-specific ecotoxicological data were not available for o-xylene, the ERLs for surface water and drinking water are taken as substitute (Van Vlaardingen and Verbruggen, 2007).

3.2.6.1 MPC$_{eco, gw}$

The MPC$_{eco, gw}$ is equal to the MPC$_{eco,water}$ of 4.10 µg/L

3.2.6.2 MPC$_{human, gw}$

The MPC$_{human, gw}$ is equal to the MPC$_{dw, water}$ of 525 µg/L.

3.2.6.3 MPC$_{gw}$

The lowest value of the routes included is the MPC$_{eco, gw}$ (see section 2.3). Therefore, the MPC$_{gw}$ is 4.10 µg/L.

3.2.6.4 NC$_{gw}$

According to Van Vlaardingen and Verbruggen (2007), the NC should be *'set to a factor of 100 below the MPC, which defines a safety margin allowing for combination toxicity.'* Thus, the NC$_{gw}$ for o-xylene is the MPC$_{gw}$ of 4.10 µg/L / 100 = 0.04 µg/L.

3.2.7 Derivation of ERL for air

3.2.7.1 MPC$_{human, air}$

According to Van Vlaardingen and Verbruggen (2007): *'Human exposure via air is covered via the Tolerable Concentration in Air (TCA). The TCA is an existing standard (µg/m^3) aimed at the protection of humans from deleterious effects after continuous lifetime exposure via air.'*
In 2001, a TCA of 870 µg/m^3 was derived (Baars et al., 2001). Thus, the MPC$_{human, air}$ is 870 µg/m^3.

3.2.8 Comparison of derived ERLs with monitoring data

An overview of the derived ERLs is given in Table 18.

Table 18. Derived MPC, NC, MAC_{eco}, and SRC_{eco} values for o-xylene.

ERL	Unit	MPC	MAC_{eco}	NC	SRC
Freshwater[a]	µg/L	4.10	41.0	0.04	1000
Marine water	µg/L	0.41	8.2	0.004	n.a.[b]
Soil	µg/kg	56.0	n.a.[b]	0.56	n.d.[a]
Groundwater	µg/L	4.10	n.a.[b]	0.04	n.a.[b]
Air	$\mu g/m^3$	870	n.a.[b]	n.a.[b]	n.a.[b]

[a] n.d. = not derived.

[b] n.a. = not applicable.

Monitoring data for the Rhine from the years 2001-2006, obtained from RIWA (Association of River Waterworks), show that at all sampling occasions and locations, the concentration of o-xylene in water was below detection limits (0.02 µg/L).

3.3 p-xylene

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

3.3.1.1 Identity

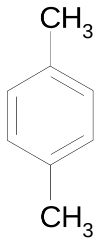

Figure 3. Structural formula of p-xylene.

Table 19. Identification of p-xylene.

Parameter	Name or number	Source
Chemical name	1,4-dimethylbenzene	Mackay et al., 2006
Common/trivial/other name	para-xylene, p-xylol, 4-methyltoluene	Mackay et al., 2006
CAS number	106-42-3	Mackay et al., 2006
EC number	203-396-5	
SMILES code	Cc1ccc(C)cc1	

3.3.1.2 Physico-chemical properties

Table 20. Physico-chemical properties of p-xylene.

Parameter	Unit	Value	Remark	Reference
Molecular weight	[g/mol]	106.165		Mackay et al., 2006
Water solubility	[mg/L]	191	20°C, shake flask	Mackay et al., 2006
log K_{OW}	[-]	3.15		Mackay et al., 2006
log K_{OC}	[-]	2.37	HPLC scr. meth.	Mackay et al., 2006
Vapour pressure	[Pa]	787	20°C	Mackay et al., 2006
Melting point	[°C]	13.25		Mackay et al., 2006
Boiling point	[°C]	138.37		Mackay et al., 2006
Henry's law constant	[Pa.m^3/mol]	754	EPIC-GC-FID	Mackay et al., 2006

n.a. = not applicable.

3.3.1.3 Behaviour in the environment

Table 21. Selected environmental properties of p-xylene.

Parameter	Unit	Value	Remark	Reference
Hydrolysis half-life	DT50 [d]		no hydrolysable functional groups	Mackay et al., 2006

In water, volatilisation seems to be the dominant removal process with a half-life of 3.1 hours (depth 1m, wind speed 3 m/s, current 1 m/s) Mackay et al., 2006.

3.3.1.4 Bioconcentration and biomagnification

An overview of the bioaccumulation data for p-xylene is given in Table 22. Detailed bioaccumulation data for p-xylene are tabulated in Appendix 1.

Table 22. Overview of bioaccumulation data for p-xylene.

Parameter	Unit	Value	Remark	Reference
BCF (fish)	[L/kg]	23.6	Exposure in crude oil suspension	Ogata and Miyake, 1978
BMF	[kg/kg]	1	Default value for BCF < 2000 L/kg	

3.3.1.5 Human toxicological threshold limits and carcinogenicity

The following R-phrases were assigned to p-xylene: R10, R20/21, R38. P-xylene is not classified as being a carcinogen. The Tolerable Daily Intake (TDI) for xylenes is 150 μg/kg bw day (Baars et al., 2001).

3.3.2 Trigger values.

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

Table 23. p-xylene: collected properties for comparison to MPC triggers.

Parameter	Value	Unit	Method/Source	Derived at section
Log $K_{p,susp-water}$	1.37	[-]	$K_{OC} \times f_{OC,susp}$[1]	K_{OC}: 3.1.1.2
BCF	23.6	[L/kg]		3.1.1.4
BMF	1	[kg/kg]		3.1.1.4
Log K_{OW}	3.15	[-]		3.1.1.2
R-phrases	R10, R20/21, R38	[-]		3.1.1.5
A1 value	not available	[μg/L]		
DW standard	not available	[μg/L]		

1 $f_{OC,susp} = 0.1\ kg_{OC}/kg_{solid}$ (EC, 2003).

o

o p-xylene has a log $K_{p,\ susp,\ water} < 3$; derivation of $MPC_{sediment}$ is not triggered.

o p-xylene has a log $K_{psusp,\ water} < 3$; expression of the MPC_{water} as $MPC_{susp,\ water}$ is not required.

o p-xylene has a BCF < 100 L/kg; assessment of secondary poisoning is not triggered.

o For p-xylene, no A1 and no Drinking Water Standard are available from Council Directives 75/440, EEC and 98/83/EC, respectively. Therefore, a provisional DWS needs to be derived.

3.3.3 Toxicity data and derivation of ERLs for water

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

An overview of the selected toxicity data for p-xylene is given in Table 24 (freshwater) and Table 25 (marine water). Detailed toxicity data for p-xylene are tabulated in Appendix 2.

Table 24. P-xylene: selected freshwater toxicity data for ERL derivation.

Chronic[a] **Taxonomic group**	**NOEC/EC10 (mg/L)**	**Acute**[a] **Taxonomic group**	**L(E)C50 (mg/L)**
Algae		Algae	
Pseudokirchneriella subcapitata	0.91[b]	*Pseudokirchneriella subcapitata*	3.74[c]
		Scenedesmus quadricauda	9.56
		Crustacea	
		Daphnia magna	12.16[d]
		Daphnia spinulata	4.25
		Hyalella curvispina	4.25
		Pisces	
		Bryconamericus iheringii	6.63[e]
		Cnesterodon decemmaculatus	6.17
		Oncorhynchus mykiss	**2.60**
		Pimephales promelas	8.91
		Poecilia reticulata	8.80

[a] For detailed information see Appendix 2. Bold values are used for ERL derivation.
[b] Geometric mean of 0.9, 0.44 and 1.90 mg/L; parameter growth.
[c] Geometric mean of 3.20 and 4.36 mg/L; parameter growth..
[d] Geometric mean of 32.24, 8.49, 3.60 and 22.18 mg/L.
[e] Geometric mean of 6.37 and 6.90 mg/L.

Table 25. P-xylene: selected marine toxicity data for ERL derivation.

Chronic [a] **Taxonomic group**	**NOEC/EC10 (mg/L)**	**Acute** [a] **Taxonomic group**	**L(E)C50 (mg/L)**
		Bacteria	
		Vibrio fischeri	17.22
		Crustacea	
		Artemia salina	27.80

[a] For detailed information see Appendix 2. Bold values are used for risk assessment.

3.3.3.2 Treatment of fresh- and saltwater toxicity data

The datasets were compared according to the guidance of Van Vlaardingen and Verbruggen (2007). Based on the result of the t-test (α >0.05), the fresh- and saltwater data can be combined.

3.3.3.3 Mesocosm studies

No mesocosm studies are available for p-xylene.

3.3.3.4 Derivation of $MPC_{eco,\ water}$ and $MPC_{eco,\ marine}$

Freshwater

The base set is complete. However, since only one chronic NOEC for algae (0.91 mg/L) was available an assessment factor of 1000 should be used on the lowest $L(E)C_{50}$ value, resulting in a $MPC_{eco,\ water}$ of 2.60 mg/L / 1000 = 2.60 µg/L.

Marine water

Since the datasets for freshwater can be combined, the $MPC_{eco,\ marine}$ is 2.60 mg/L / 10000 = 0.26 µg/L.

3.3.3.5 $MPC_{sp,\ water}$ and $MPC_{sp,\ marine}$

P-xylene has a BCF<100 L/kg, thus assessment of secondary poisoning is not triggered.

3.3.3.6 $MPC_{hh\ food,\ water}$

Derivation of $MPC_{hh\ food,\ water}$ for p-xylene is not triggered (Table 23).

3.3.3.7 $MPC_{dw,\ water}$

For p-xylene, no A1 and no Drinking Water Standard are available from Council Directives 75/440, EEC and 98/83/EC, respectively. Therefore, a provisional DWS based on the TDI value for xylenes (150 µg/kg$_{bw}$ day Baars et al., 2001) should be derived, resulting in a $MPC_{dw\ ,water}$ of 525 µg/L (Van Vlaardingen and Verbruggen 2007, section 3.1.6).

3.3.3.8 $MPC_{humn,\ water}$

Following WFD methodology, the derivation of the $MPC_{human,\ water}$ is integrated in the MPC derivation for the water compartment. Since derivation of the $MPC_{hh\ food,\ water}$ for p-xylene is not triggered (Table 23), the $MPC_{huamn,gw}$ is equal to the $MPC_{dw,water}$ of 525 µg/L (Van Vlaardingen and Verbruggen, 2007).

Thus, the $MPC_{human,water}$ is 525 µg/L.

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

Freshwater

The lowest value of the routes included is the $MPC_{eco,water}$ (see section 2.3). Therefore, the MPC_{water} is 2.60 µg/L.

Marine water

The lowest value of the routes included is the $MPC_{eco,marine}$ (see section 2.3). Therefore, the MPC_{marine} is 0.26 µg/L.

3.3.3.10 $MAC_{eco,\ water}$

Since the base set for p-xylene is complete, the substance does not bioaccumulate (BCF<100 L/kg) and the mode of toxic action is known (nonpolar narcosis), an assessment factor of 100 can be used for the derivation of the $MAC_{eco,\ water}$. The lowest LC_{50} value of 2.60 mg/L for the fish *Oncorhynchus mykiss* results in a $MAC_{eco,\ water}$ of 2.60 mg/L / 100 = 26.0 µg/L.

3.3.3.11 $MAC_{eco,\ marine}$

Since the datasets for freshwater and marine water can be combined an no information about toxicity of p-xylene for specific marine taxonomic groups is available, the $MAC_{eco,\ marine}$ is derived by applying an additional assessment factor of 10 on the $MAC_{eco,water}$. Thus, the $MAC_{eco,\ marine}$ is 26.0 µg/L / 10 = 2.60 µg/L.

3.3.3.12 NC$_{water}$

According to Van Vlaardingen en Verbruggen (2007), the NC should be *'set to a factor of 100 below the MPC, which defines a safety margin allowing for combination toxicity.'* Thus, the NC$_{water}$ for p-xylene is the MPC$_{water}$ of 2.60 μg/L / 100 = 0.03 μg/L.

3.3.3.13 NC$_{marine}$

According to Van Vlaardingen en Verbruggen (2007), the NC should be *'set to a factor of 100 below the MPC, which defines a safety margin allowing for combination toxicity.'* Thus, the NC$_{marine}$ for p-xylene is the MPC$_{marine}$ of 0.26 μg/L / 100 = 0.003 μg/L.

3.3.3.14 SRC$_{eco}$

The base set is complete and one NOEC for algae (0.91 mg/L) is available. The datasets for freshwater and marine water were combined. The geometric mean of the combined LC$_{50}$ values is 7.49 mg/L. Since this geometric mean is less than 10 times higher than the NOEC, the SRC$_{eco}$ is based on the geometric mean of the LC$_{50}$ values using an assessment factor of 10. The SRC$_{eco}$ for p-xylene is 7.49 mg/L / 10 = 749 μg/L.

3.3.4 Toxicity data and derivation of ERLs for sediment

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

3.3.5 Toxicity data and derivation of ERLs for soil

3.3.5.1 MPC$_{eco,\ soil}$

Because no soil data for p-xylene are available, the equilibrium partitioning method is used (Van Vlaardingen and Verbruggen, 2007, section 3.7). Using K$_{air\text{-}water}$ = 0.32 m^3/m^3, Kp$_{soil}$ = 4.7 L/kg, K$_{soil\text{-}water}$ = 7.30, the MPC$_{Dutch\ standard\ soil,\ EqP,\ dwt}$ is calculated to be 37.2 μg/kg.

3.3.5.2 MPC$_{sp,\ soil}$

p-xylene has a BCF $<$ 100 L/kg, thus assessment of secondary poisoning is not triggered.

3.3.5.3 MPC$_{human,\ soil}$

According to the methods in the INS Guidance (Van Vlaardingen and Verbruggen, 2007, section 3.3.6), the MPC$_{human,\ soil}$ is 1.853 mg/kg$_{dwt}$ = 1853 μg/kg for the consumption of root crops.

3.3.5.4 NC$_{soil}$

According to Van Vlaardingen en Verbruggen (2007), the NC should be *'set to a factor of 100 below the MPC, which defines a safety margin allowing for combination toxicity.'* Thus, the NC$_{soil}$ for p-xylene is the MPC$_{soil}$ of 37.2 μg/kg / 100 = 0.37 μg/kg.

3.3.5.5 SRC$_{soil}$

Since no toxicity data are available, the SRC$_{soil}$ can not be derived.

3.3.6 Derivation of ERLs for groundwater

Since groundwater-specific ecotoxicological data are not available for p-xylene, the ERLs for surface water and drinking water are taken as substitute (Van Vlaardingen and Verbruggen, 2007).

3.3.6.1 $MPC_{eco, gw}$

The $MPC_{eco, gw}$ is equal to the $MPC_{eco,water}$ of 2.60 µg/L.

3.3.6.2 $MPC_{human, gw}$

The $MPC_{human, gw}$ is equal to the $MPC_{dw, water}$ of 525 µg/L.

3.3.6.3 MPC_{gw}

The lowest value of the routes included is the $MPC_{eco, gw}$ (see section 2.3). Therefore, the MPC_{gw} is 2.60 µg/L.

3.3.6.4 NC_{gw}

According to Van Vlaardingen and Verbruggen (2007), the NC should be *'set to a factor of 100 below the MPC, which defines a safety margin allowing for combination toxicity.'* Thus, the NC_{gw} for p-xylene is the MPC_{gw} of 2.60 µg/L / 100 = 0.03 µg/L.

3.3.7 Derivation of ERL for air

3.3.7.1 $MPC_{human, air}$

According to Van Vlaardingen and Verbruggen (2007): *'Human exposure via air is covered via the Tolerable Concentration in Air (TCA). The TCA is an existing standard (µg/m^3) aimed at the protection of humans from deleterious effects after continuous lifetime exposure via air.'*
In 2001, a TCA of 870 µg/m^3 was derived (Baars et al., 2001). Thus, the $MPC_{human, air}$ is 870 µg/m^3.

3.3.8 Comparison of derived ERLs with monitoring data

An overview of the derived ERLs is given in Table 26.

Table 26. Derived MPC, NC, MAC_{eco}, and SRC_{eco} values for p-xylene.

ERL	Unit	MPC	MAC_{eco}	NC	SRC
Freshwater[a]	µg/L	2.60	26.0	0.03	749
Marine water	µg/L	0.26	2.60	0.003	n.a.[b]
Soil	µg/kg	37.2	n.a.[b]	0.37	n.d.[a]
Ground water	µg/L	2.60	n.a.[b]	0.03	n.a.[c]
Air	µg/m^3	870	n.a.[b]	n.a.[b]	n.a.[c]

[a] n.d. = not derived.

[b] n.a. = not applicable.

Monitoring data for the Rhine from the years 2001-2006, obtained from RIWA (Association of River Waterworks), show that at all sampling occasions and locations, the concentration of p-xylene in water was below detection limits (0.02 µg/L).

3.4 Xylene (grouped isomers)

Since the differences in toxicity for the individual xylene isomers are small, additional environmental risk limits were derived for the xylenes as a group based on the combined datasets of m-, o- and p-xylene. Only ERLs which are relevant for the individual xylene isomers are also derived for the grouped isomers.

3.4.1 Toxicity data and derivation of ERLs for water

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

An overview of the selected toxicity data for xylene is given in Table 27 (freshwater) Table 28 (marine water). Detailed toxicity data for xylene are tabulated in Appendix 2. Note that the aggregated data table for the grouped isomers differs from those for the individual isomers due to the larger amount of data on which the geometric means are based.

Table 27. Xylene: selected freshwater toxicity data for ERL derivation.

Chronic[a]		**Acute[a]**	
Taxonomic group	**NOEC/EC10 (mg/L)**	**Taxonomic group**	**L(E)C50 (mg/L)**
Algae		Algae	
Chlorella vulgaris	12.47	*Pseudokirchneriella subcapitata*	4.23[c]
Pseudokirchneriella subcapitata	**0.86**[b]	*Scenedesmu quadricauda*	12.52[d]
		Crustacea	
		Cerodaphnia cf. dubia	**2.44**
		Daphnia magna	7.32[e]
		Daphnia spinulata	4.86[f]
		Hyalella curvispina	4.86[g]
		Pisces	
		Bryconamericus iheringii	9.04[h]
		Carassius auratus	16.10
		Cataostomus commersoni	16.10
		Cnesterodon decemmaculatus	8.51[i]
		Lepomis macrochirus	16.10
		Oncorhynchus mykiss	6.05[j]
		Oryzias latipes	32.00
		Pimephales promelas	17.51[k]
		Poecilia reticulata	11.09[l]

[a] For detailed information see Appendix 2. Bold values are used for ERL derivation.

[b] Geometric mean of 0.7, 0.9 and 1.0 mg/L.

[c] Geometric mean of 3.20, 4.36, 4.70 and 4.90 mg/L.

[d] Geometric mean of 7.43, 9.56 and 27.60 mg/L.

[e] Geometric mean of 1.00, 3.60, 4.70, 17.22, 22.18 and 23.77 mg/L.

[f] Geometric mean of 4.25, 4.25 and 6.37 mg/L.

[g] Geometric mean of 4.25, 4.25 and 6.37 mg/L.

[h] Geometric mean of 6.37, 6.90, 9.56, 9.94, 11.23 and 11.68 mg/L.

[i] Geometric mean of 6.17, 9.33 and 10.72 mg/L.

[j] Geometric mean of 2.60, 7.60, 8.05 and 8.40 mg/L.

[k] Geometric mean of 8.91, 15.49, 16.22 and 42.00 mg/L.
[l] Geometric mean of 8.80, 12.00 and 12.90 mg/L.

Table 28. Xylene: selected marine toxicity data for ERL derivation.

Chronic[a] **Taxonomic group**	**NOEC/EC10 (mg/L)**	**Acute**[a] **Taxonomic group**	**L(E)C50 (mg/L)**
		Bacteria	
		Vibrio fischeri	12.84[b]
		Crustacea	
		Artemia salina	16.31[c]
		Echinodermata	
		Strongylocentrotus droebachiensis	**4.10**

[a] For detailed information see Appendix 2. Bold values are used for ERL derivation.
[b] Geometric mean of 8.83, 9.25, 17.22 and 19.31 mg/L.
[c] Geometric mean of 10.80 and 24.64 mg/L.

3.4.1.2 Treatment of fresh- and saltwater toxicity data

The datasets were compared according to the guidance of Van Vlaardingen and Verbruggen (2007). Based on the result of the t-test ($\alpha > 0.05$), the fresh- and saltwater data can be combined.

3.4.1.3 Derivation of $MPC_{eco, water}$ and $MPC_{eco, marine}$

Freshwater

The base set is complete, two chronic NOECs were available for algae. Therefore, an assessment factor of 1000 is used on the lowest $L(E)C_{50}$ value of 2.44 mg/L for *Ceriodaphnia cf. dubia*. This results in a $MPC_{eco, water}$ of 2.44 mg/L /1000 = 2.44 µg/L

Marine water

Since the datasets for freshwater can be combined, the $MPC_{eco,marine}$ is also based on the $L(E)C_{50}$ for *Ceriodaphnia cf. dubia* using an assessment factor of 10000. The $MPC_{eco, marine}$ is 2.44 mg/L /10000 = 0.24 µg/L.

3.4.1.4 $MPC_{dw,water}$

For p-xylene, no A1 and no Drinking Water Standard are available from Council Directives 75/440, EEC and 98/83/EC, respectively. Therefore, a provisional DWS based on the TDI value for xylenes (150 µg/kg bw day Baars et al., 2001) should be derived, resulting in a $MPC_{dw,water}$ of 525 µg/L (Van Vlaardingen and Verbruggen 2007, section 3.1.6).

3.4.1.5 $MPC_{human, water}$

Following WFD methodology, the derivation of the $MPC_{human, water}$ is integrated in the MPC derivation for the water compartment. Since derivation of the $MPC_{hh\ food, water}$ for xylene is not triggered, the $MPC_{huamn,gw}$ is equal to the $MPC_{dw,water}$ of 525 µg/L (Van Vlaardingen and Verbruggen, 2007).

3.4.1.6 Selection of the $\mathrm{MPC_{water}}$ and $\mathrm{MPC_{marine}}$

Freshwater

In the Fraunhofer document (Lepper, 2005) it is prescribed that the lowest MPC value should be selected as the general MPC. The lowest value of the routes included is the $\mathrm{MPC_{eco,\ water}}$. Therefore, the $\mathrm{MPC_{water}}$ is 2.44 µg/L.

Marine water

In the Fraunhofer document (Lepper, 2005) it is prescribed that the lowest MPC value should be selected as the general MPC. The lowest value of the routes included is the $\mathrm{MPC_{eco,\ marine}}$. Therefore, the $\mathrm{MPC_{marine}}$ is 0.24 µg/L.

3.4.1.7 $\mathrm{MAC_{eco,\ water}}$

Since the base set for xylene is complete, the substance does not bioaccumulate (BCF<100 L/kg) and the mode of toxic action is known (nonpolar narcosis), an assessment factor of 100 can be used for the derivation of the $\mathrm{MAC_{eco,\ water}}$. The lowest $\mathrm{EC_{50}}$ value of 2.44 mg/L for *Cerodaphnia cf. dubia* results in a $\mathrm{MAC_{eco,water}}$ of 2.44 mg/L / 100 = 24.4 µg/L.

3.4.1.8 $\mathrm{MAC_{eco,\ marine}}$

Since the datasets for freshwater and marine water can be combined and information is available on an specific marine taxonomic group, the $\mathrm{MAC_{eco,\ marine}}$ is derived by applying assessment factor of 500 on the $\mathrm{EC_{50}}$ value for *Cerodaphnia cf. dubia*. Thus, the $\mathrm{MAC_{eco,marine}}$ is 2.44 mg/L /500 = 4.88 µg/L.

3.4.1.9 $\mathrm{NC_{water}}$

According to Van Vlaardingen en Verbruggen (2007), the NC should be *'set to a factor of 100 below the MPC, which defines a safety margin allowing for combination toxicity.'* Thus, the $\mathrm{NC_{water}}$ for xylene is the $\mathrm{MPC_{water}}$ of 2.44 µg/L / 100 = 0.02 µg/L.

3.4.1.10 $\mathrm{NC_{marine}}$

In accordance with the method described above, the $\mathrm{NC_{marine}}$ for xylene is the $\mathrm{MPC_{marine}}$ of 0.24 µg/L / 100 = 0.002 µg/L.

3.4.1.11 $\mathrm{SRC_{eco}}$

The base set is complete and two NOEC values for algae (0.86 and 12.47 mg/L, geometric mean 3.27 mg/L) are available. The datasets for freshwater and marine water were combined. The geometric mean of the combined $\mathrm{LC_{50}}$ values is 9.22 mg/L. Since this geometric mean is less than 10 times higher than the geometric mean of the NOEC values, the $\mathrm{SRC_{eco}}$ is based on the geometric mean of the $\mathrm{LC_{50}}$ values using an assessment factor of 10. The $\mathrm{SRC_{eco}}$ for p-xylene is 9.22 mg/L / 10 = 922 µg/L.

3.4.2 Toxicity data and derivation of ERLs for soil

3.4.2.1 $\mathrm{MPC_{eco,\ soil}}$

Because no soil data for xylene are available, the equilibrium partitioning method is used (Van Vlaardingen and Verbruggen, 2007, section 3.7). Using a log Koc of 2.35 and a Henry's law constant of 651 $\mathrm{Pa.m^3/mol}$, this results in a $\mathrm{MPC_{Dutch\ standard\ soil,\ EqP,\ dwt}}$ of 33.35 µg/kg soil.

3.4.2.2 $\mathrm{MPC_{human,\ soil}}$

According to the methods in the INS Guidance (Van Vlaardingen and Verbruggen, 2007, section 3.3.6), the $\mathrm{MPC_{human,\ soil\ dwt}}$ is 1.851 mg/kg = 1851 µg/kg.

3.4.2.3 MPC$_{soil}$

The lowest value of the routes included is the MPC$_{eco,soil}$ (see section 2.3). Therefore, the MPC$_{soil}$ is 33.35 µg/L.

3.4.2.4 NC$_{soil}$

According to Van Vlaardingen en Verbruggen (2007), the NC should be *'set to a factor of 100 below the MPC, which defines a safety margin allowing for combination toxicity.'* Thus, the NC$_{soil}$ for xylene is the MPC$_{soil}$ of 33.35 µg/kg / 100 = 0.33 µg/kg.

3.4.3 Derivation of ERLs for groundwater

Since groundwater-specific ecotoxicological data are not available for xylene, the ERLs for surface water and drinking water are taken as substitute (Van Vlaardingen and Verbruggen, 2007).

3.4.3.1 MPC$_{eco,gw}$

The MPC$_{eco,gw}$ is equal to the MPC$_{eco,water}$ of 2.44 µg/L.

3.4.3.2 MPC$_{human,gw}$

The MPC$_{human,gw}$ is equal to the MPC$_{dw,water}$ of 525 µg/L.

3.4.3.3 MPC$_{gw}$

The lowest value of the routes included is the MPC$_{eco,gw}$ (see section 2.3). Therefore, the MPC$_{gw}$ is 2.44 µg/L.

3.4.3.4 NC$_{gw}$

According to Van Vlaardingen and Verbruggen (2007), the NC should be *'set to a factor of 100 below the MPC, which defines a safety margin allowing for combination toxicity.'* Thus, the NC$_{gw}$ for xylene is the MPC$_{gw}$ of 2.44 µg/L / 100 = 0.02 µg/L.

3.4.4 Derivation of ERL for air

3.4.4.1 MPC$_{human, air}$

According to Van Vlaardingen and Verbruggen (2007): *'Human exposure via air is covered via the Tolerable Concentration in Air (TCA). The TCA is an existing standard (µg/m^3) aimed at the protection of humans from deleterious effects after continuous lifetime exposure via air.'*
In 2001, a TCA of 870 µg/m^3 was derived (Baars et al., 2001). Thus, the MPC$_{human, air}$ is 870 µg/m^3.

3.4.5 Comparison of derived ERLs with monitoring data

An overview of the derived ERLs is given in Table 29.

Table 29. Derived MPC, NC, MAC$_{eco}$, and SRC$_{eco}$ values for xylene (grouped isomers).

ERL	Unit	MPC	MAC	NC	SRC
Freshwater	µg/L	2.44	24.4	0.02	922
Marine water	µg/L	0.24	4.88	0.002	n.a.[b]
Soil	µg/kg	33.35	n.a.[b]	0.33	n.d.[a]
Ground water	µg/L	2.44	n.a.[b]	0.02	n.a.[b]
Air	µg/m^3	870	n.a.[b]	n.a.[c]	n.a.[b]

[a] n.d. = not derived.

[b] n.a. = not applicable.

Monitoring data for the Rhine from the years 2001-2006, obtained from RIWA (Association of River Waterworks), show that at all sampling occasions and locations, the concentration of m-, o-, and p-xylene in water was below detection limits (0.02 µg/L). Based on these data and the physico-chemical properties of the substance, the new MPC is not expected to be exceeded.

3.5 Sum limits

Since the differences in toxicity for the individual xylene isomers are small, additional environmental risk limits were derived for the xylenes as a group based on the combined datasets of m-, o- and p-xylene.

These ERLs differ less than a factor of 3 from the ERLs derived for the individual isomers, potentially resulting in unacceptable risks when a mixture of xylene isomers is present at one location. In order to prevent this accumulation of toxicity, the use of a sum limit for the xylene isomers is proposed. In this approach, the sum of the concentrations of the combination of the three individual isomers should not exceed the ERLs for the grouped xylene isomers (Table 29). It should be noted that the sum limit only applies when all three isomers are monitored.

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 m-xylene, o-xylene, p-xylene and xylene (mixed isomers) in water, groundwater and soil. 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.

Table 30. Derived MPC, NC, MAC_{eco}, and SRC values.

ERL	Unit	Substance	MPC	MAC	NC	SRC
Freshwater	µg/L	m-xylene	2.44	24.4	0.24	700
Marine water	µg/L	m-xylene	0.24	2.44	0.02	n.a.[b]
Soil	µg/kg	m-xylene	31.9	n.a.[b]	0.32	n.d.[a]
Groundwater	µg/L	m-xylene	2.44	n.a.[b]	0.02	n.a.[b]
Air	µg/m^3	m-xylene	870	n.a.[b]	n.a.[b]	n.a.[b]
Freshwater	µg/L	o-xylene	4.10	41.0	0.04	1000
Marine water	µg/L	o-xylene	0.41	8.2	0.004	n.a.[b]
Soil	µg/kg	o-xylene	56.0	n.a.[b]	0.56	n.d.[a]
Groundwater	µg/L	o-xylene	4.10	n.a.[b]	0.04	n.a.[b]
Air	µg/m^3	o-xylene	870	n.a.[b]	n.a.[b]	n.a.[b]
Freshwater	µg/L	p-xylene	2.60	26.0	0.03	749
Marine water	µg/L	p-xylene	0.26	2.60	0.003	n.a.[b]
Soil	µg/kg	p-xylene	37.2	n.a.[b]	0.37	n.d.[a]
Ground water	µg/L	p-xylene	2.60	n.a.[b]	0.03	n.a.[b]
Air	µg/m^3	p-xylene	870	n.a.[b]	n.a.[b]	n.a.[b]
Freshwater	µg/L	xylene	2.44	24.4	0.02	922
Marine water	µg/L	xylene	0.24	4.88	0.002	n.a.[b]
Soil	µg/kg	xylene	33.35	n.a.[b]	0.33	n.d.[a]
Ground water	µg/L	xylene	2.44	n.a.[b]	0.02	n.a.[b]
Air	µg/m^3	xylene	870	n.a.[b]	n.a.[b]	n.a.[b]

[a] n.d. = not derived due to lack of data

[b] n.a. = not applicable

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Appendix 1. Information on bioconcentration

Table A1.1 Bioconcentration of m-xylene

Species	Species properties	Substance purity (%)	Analysed	Test type	Test water	pH	Hardness/ Salinity [g/l]	Temp [°C]	Exposure time	Exp. conc. [mg/l]	BCF [l/kg$_{w.w.}$]	Method	Validity	Notes	Reference
Algae															
Pseudokirchneriella subcapitata			GC			23			12h	8,33	251.19	micro-extraction, GC	3	1,2	Herman et al., 1991
Scenedesmus quadricauda		GC standard	GC-FID	S	am	7.5		22	96h		37.65		2	3	Di Marzio and Saenz, 2006
Crustacea															
Daphnia spinulata	< 24h	GC standard	GC-FID	S	am	7.8	95.8	20	48h		63.96		2	3	Di Marzio and Saenz, 2006
Hyalella curvispina	10 day	GC standard	GC-FID		dw	8.3	126	21	96h		62.90		2	3	Di Marzio and Saenz, 2006
Mollusca															
Tapes semidecussata			GC-FID	CF			30	14	8d	3,1	6.43		2	4	Nunes and Benville, 1979
Pisces															
Anguilla japonica	130-180g		GC-FID					20	10d	50	23.6		2	3	Ogata and Miyake, 1978
Carassius auratus			GC-FID	S?						1	14.79		4	5	Ogata et al, 1984

Notes

1	Recalculated from ug/kg
2	BTEX mixture used for exposure
3	Exposure in crude oil suspension
4	Water is filtered and sterilized using UV light, exposure 3,1ppm, analysis 3x/day
5	No data on or exp. time, logBCF=1,17

Table A1.2 Bioconcentration of o-xylene

Species	Species properties	Substance purity (%)	Analysed	Test type	Test water	pH	Hardness/ Salinity [g/l]	Temp [°C]	Exposure time	Exp. conc. [mg/l]	BCF [l/kg$_{w.w.}$]	Method	Validity	Notes	Reference
Algae															
Pseudokirchneriella subcapitata			GC			23			12h	8,33	218.78		3	1, 2	Herman et al, 1991
Scenedesmus quadricauda		GC standard	GC-FID	S	am	7.5		22	96h		9.76		2	3	Di Marzio and Saenz, 2006
Crustacea															
Daphnia spinulata	< 24h	GC standard	GC-FID	S	am	7.8	95.8	20	48h		43.44		2	3	Di Marzio and Saenz, 2006
Hyalella curvispina	10 day	GC standard	GC-FID		dw	8.3	126	21	96h		42.60		2	3	Di Marzio and Saenz, 2006
Mollusca															
Tapes semidecussata			GC-FID	CF			30	14	8d	3,1	7.25		2	4	Nunes and Benville, 1979
Pisces															
Anguilla japonica	130-180g		GC-FID					20	10d	50	21.4		2	3	Ogata and Miyake, 1978
Carassius auratus			GC-FID	S?						1	14.13		4	5	Ogata et al, 1984

Notes

1	Recalculated from ug/kg
2	BTEX mixture used for exposure
3	Exposure in crude oil suspension
4	Water is filtered and sterilized using UV light, exposure 3,1ppm, analysis 3x/day
5	No data on or exp. time, logBCF=1,17

Table A1.3 Bioconcentration of p-xylene

Species	Species properties	Substance purity (%)	Analysed	Test type	Test water	pH	Hardness/ Salinity [g/l]	Temp [°C]	Exposure time	Exp. conc. [mg/l]	BCF [l/kg$_{w.w.}$]	Method	Validity	Notes	Reference
Algae															
Pseudokirchneriella subcapitata			GC			23			12h	8,33	257.04		3	1,2	Herman et al, 1991
Scenedesmus quadricauda		GC standard	GC-FID	S	am	7.5		22	96h		26.60		2	3	Di Marzio and Saenz, 2006
Crustacea															
Daphnia spinulata	< 24h	GC standard	GC-FID	S	am	7.8	95.8	20	48h		60.60		2	3	Di Marzio and Saenz, 2006
Hyalella curvispina	10 day	GC standard	GC-FID		dw	8.3	126	21	96h		58.34		2	3	Di Marzio and Saenz, 2006
Pisces															
Anguilla japonica	130-180g		GC-FID					20	10	50	23.6		2	5	Ogata and Miyake, 1978
Carassius auratus			GC-FID	S?						1	14.79		4	4	Ogata et al, 1984

Notes

1	Recalculated from ug/kg
2	BTEX mixture used for exposure
3	Exposure in crude oil suspension
4	No data on or exp. time, logBCF=1,17

Appendix 2. Detailed aquatic toxicity data

Table A2.1. Acute toxicity of m-xylene to freshwater organisms.

Species	Species properties	A	Test type	Purity [%]	Test water	pH	T [°C]	Hardness [mg $CaCO_3$/l]	Exp. time	Criterion	Test endpoint	Value [mg/l]	Validity	Notes	Reference
Protozoa															
Tetrahymena pyriformis	stat. phase		S		am		28	20	24h	LC100	Mortality	399.60	3	3,17	IUCLID 2000: Schultz et al, 1978
Algae															
Scenedesmus quadricauda		y	S	GC std.	am	7.5	22		96h	EC50	Growth	7.43	2	4,6,8	Di Marzio and Saenz, 2006
Pseudokirchneriella subcapitata	log phase		S		am	7			8d	EC50	Growth	3.90	3	7	IUCLID 2000: Herman, 1990
Pseudokirchneriella subcapitata		n	Sc?	GC std.					72h	EC50	Growth	4.90	3	2,4,8	Galassi et al, 1998
Crustacea															
Cerodaphnia cf. dubia		y	Sc	>97		7.7		65.2	48h	EC50	Immobilisation	2.44	2	9,10,11	Rose et al, 1998
Daphnia magna	24h	y	Sc		am	7.2-8	20	250	48h	LC50	Mortality	36.26	2	19	MacLean and Doe, 1989
Daphnia magna	juvenile (4-6 day)		S			6-7	23		48h	LC50	Mortality	9.56	4*		IUCLID 2000: Bobra et al 1983
Daphnia magna	4 - 6 days	n	Sc	>97	dw	6.5	23		48h	LC50	Mortality	9.55	3	12	Bobra et al, 1983
Daphnia magna		y	Sc	GC std.					24	IC50	Immobilisation	4.70	2	2,4,8	Galassi et al, 1998
Daphnia magna	6-24h old		Sc	>95	dw		22		24h	IC50	Immobilisation	23.77	2	13	Zhao, 1995
Daphnia spinulata	< 24h	y	S	GC std.	am	7.8	20	95.8	48h	LC50	Mortality	4.25	2	4,8, 14,15	Di Marzio and Saenz, 2006
Hyalella curvispina	10 day	y	S	GC std.	dw	8.3	21	82	96h	LC50	Mortality	4.25	2	4,8,15	Di Marzio and Saenz, 2006
Pisces															
Bryconamericus iheringii	4.7 cm. 2.85g	y	Sc	GC std.	nw	7.9	20	98	96h	LC50	Mortality	11.68	1	2,4, 8,16	Di Marzio and Saenz, 2006
Bryconamericus iheringii	2.85g. 4.7cm	y	Sc	GC std.					96h	LC50	Mortality	11.23	2	2,4,8	Di Marzio and Saenz, 2004
Carassius auratus									96h	LC50	Mortality	16.00	4		IUCLID 2000: Verschueren, 1983

Species	Species properties	A	Test type	Purity [%]	Test water	pH	T [°C]	Hardness [mg $CaCO_3$/l]	Exp. time	Criterion	Test endpoint	Value [mg/l]	Validity	Notes	Reference
Carassius auratus	6.2 cm.	y	S		tw	6-7	20		24h	LC50	Mortality	16.00	1	1,4	Bridie et al, 1979
Cnesterodon decemmaculatus		y	Sc	GC std.	dw	8.59	19.5	141.6	96h	LC50	Mortality	10.72	2	2,4,5, 8, 18	Di Marzio et al, 2001
Oncorhynchus mykiss		y	R	GC std.			12		96h	LC50	Mortality	8.40	2	2,5,8	Galassi et al, 1998
Oryzias latipes			R		tw	7.2	20 ± 1		96 h	LC50	Mortality	32.00	2	2	Yoshioka et al, 1993
Pimephales promelas		y	Sc	GC std.					96h	LC50	Mortality	15.49	2	2,4,8	Di Marzio and Saenz, 2001
Poecilia reticulata		y	R	GC std.			21		96h	LC50	Mortality	12.90	2	2,5,8	Galassi et al, 1998
Poecilia reticulata	2-3 mos	n	R		tw		22	25	14d	LC50	Mortality	37.67	3	1	Könemann, 1981

Notes

1 System not closed, no prevention of volatilisation
2 According to OECD guidelines
3 LC 100 value reported
4 Concentrations measured at beginning and end of test
5 Concentrations measured at renewals
6 Recalculated from 0,07 mM
7 Photoperiod 16 hours
8 Mean measured concentrations
9 According to US EPA standards
10 GC quantification
11 Recalculated from 23 umol/L
12 Recalculated from mmol/m3
13 Recalculated from 3,74 log1/value (mol/l); 14h light, 10h dark
14 Artificial pond water
15 Recalculated from 0,04 mM
16 Recalculated from 0,11 mM
17 Value exceeds water solubility
18 Recalculated from Log1/LC50 (mg/l)
19 Geomean of 23,6 and 55,7

Table A2.2. Acute toxicity of m-xylene to marine organisms.

Species	Species properties	A	Test type	Purity [%]	Test water	pH	T [°C]	Salinity [‰]	Exp. time	Criterion	Test endpoint	Value [mg/l]	Validity	Notes	Reference
Bacteria															
Vibrio fischeri			Sc	>95	dw		20	3% NaCl	15m	EC50	Luminescence	19.31	2	1	Zhao, 1995
Crustacea															
Artemia salina		y	Sc		aw	8-8.3	21.5-23	30	48h	LC50	Mortality	10.80	2	5	MacLean and Doe, 1989
Artemia salina		n	Sc	>97			20	30	24h	LC50	Mortality	19.32	3	2	Abernethy et al, 1986
Crago franciscorum	1.8g	y	S	>99	nw		16	25	96h	LC50	Mortality	3.70	3	3	Benville and Korn, 1977
Pisces															
Gadus morrhua	eggs		S	>98,5	sea		4-6	34	6h	40-50% increase of mortality	Mortality	16-35	3	4	IUCLID 2000: Khorsvik et al, 1982
Morone saxatilis	6.0g	y	S	>99	nw		16	25	96h	LC50	Mortality	9.20	3	3	Benville and Korn, 1977

Notes

1	Recalculated from log1/value (3,74 mol/l)
2	Methods in Wells et al 1982, value recalculated from mmol/m3
3	>99% loss of concentration after 96h, GC analysis after 0, 24, 48, 72, 96 hours
4	Eggs were exposed 1,5 hour after fertilisation an the effect measured 17 days post-exposure
5	Geomean of 14,8, 12,2, 8,84, 8,52

Table A2.3. Chronic toxicity of m-xylene to freshwater organisms.

Species	Species properties	A	Test type	Purity [%]	Test water	pH	T [°C]	Hardness [mg $CaCO_3$/l]	Exp. time	Criterion	Test endpoint	Value [mg/l]	Validity	Notes	Reference
Algae															
Pseudokirchneriella subcapitata		y	Sc			neutral			8d	NOEC	Growth	0.7	2	1	Herman et al, 1990

Notes

1 16h/8h light/dark cycle; value based on measured concentrations; unclear when analysis is performed

Table A2.4. Acute toxicity of o-xylene to freshwater organisms.

Species	Species properties	A	Test type	Purity [%]	Test water	pH	T [°C]	Hardness [mg $CaCO_3$/l]	Exp. time	Criterion	Test endpoint	Value [mg/l]	Validity	Notes	Reference
Algae															
Pseudokirchneriella subcapitata		y	Sc?	GC std.					72h	EC50	Growth	4.70	2	1, 2, 4	Galassi et al, 1998
Scenedesmus quadricauda		y	S	GC std.	am	7.5	22		96h	EC50	Growth	27.60	2	2, 4, 8	Di Marzio and Saenz, 2006
Crustacea															
Daphnia magna	24h	y	Sc		am	7.8-8.1	19.5-22	250	48h	LC50	Mortality	17.43	2	17	MacLean and Doe, 1989
Daphnia magna	4 - 6 days	n	Sc	97	dw	6.5	23		48h	LC50	Mortality	3.18	3	5	Bobra et al, 1983
Daphnia magna		y	Sc	GC std.					24h	IC50	Immobilisation	1.00	2	1, 2, 4	Galassi et al, 1998
Daphnia magna	<24h	y	CF		nw	7.39	17	44.7	48h	LC50	Mortality	3.82	2		Holcombe et al, 1987
Daphnia magna					dw					LC50	Mortality	>100. <1000	4		Dowden and Bennett, 1965
Daphnia magna	6-24h old		Sc	>95	dw		22		24h	IC50	Immobilisation	17.22	2	9	Zhao, 1995
Daphnia spinulata	< 24h	y	S	GC std.	am	7.8	20	95.8	48h	LC50	Mortality	6.37	2	2, 4, 6, 10	Di Marzio and Saenz, 2006
Hyalella curvispina	10 day	y	S	GC std.	dw	8.3	21	82	96h	LC50	Mortality	6.37	2	2, 4, 10	Di Marzio and Saenz, 2006

Species	Species properties	A	Test type	Purity [%]	Test water	pH	T [°C]	Hardness [mg $CaCO_3$/l]	Exp. time	Criterion	Test endpoint	Value [mg/l]	Validity	Notes	Reference
Amphibiae															
Xenopus laevis	larvae		Sc		TW		20		48h	LC50	Mortality	73.00	4		IUCLID 2000: de Zwart & Slooff, 1987
Pisces															
Bryconamericus iheringii	4.7 cm. 2.85g	y	Sc	GC std.	am	7.9	20	98	96h	LC50	Mortality	9.56	1	1, 2, 4, 11	Di Marzio and Saenz, 2006
Bryconamericus iheringii	4.7 cm. 2.85g	y	Sc	GC std.					96h	LC50	Mortality	9.94	2	1, 2, 4	Di Marzio and Saenz, 2004
Carassius auratus	6.2 cm. 3.3 g	y	S		tw	6-7	20		24h	LC50	Mortality	13.00	3	2, 2	Bridie et al, 1979
Carassius auratus	2.5g	y	CF		nw	7.39	17	44.7	48h	LC50	Mortality	16.10	2	12	Holcombe et al, 1987
Catostomus commersoni	2.4g	y	CF		nw	7.39	17	44.7	48h	LC50	Mortality	16.10	2	12	Holcombe et al, 1987
Cnesterodon decemmaculatus		y	Sc	GC std.	dw	8.59	19.5	141.6	96h	LC50	Mortality	9.33	2	1, 2, 3, 4, 16	Di Marzio et al, 2001
Lepomis macrochirus	1.1	y	CF		nw	7.39	17	44.7	48h	LC50	Mortality	16.10	2	12	Holcombe et al, 1987
Oncorhynchus mykiss		y	R	GC std.			12		96h	LC50	Mortality	7.60	2	1, 3, 4	Galassi et al, 1998
Oncorhynchus mykiss	13.1g	y	CF		nw	7.39	17	44.7	48h	LC50	Mortality	8.05	2	12	Holcombe et al, 1987
Pimephales promelas	0.3	y	CF		nw	7.39	17	44.7	48h	LC50	Mortality	16.10	2	13	Holcombe et al, 1987
Pimephales promelas		y	Sc	GC std.					96h	LC50	Mortality	16.22	2	1, 2	Di Marzio and Saenz, 2001
Pimephales promelas	4-6wks. 1.1-3.1 cm	n	S		dw		18-22		96h	LC50	Mortality	42.00	3	14	Mattson et al, 1974
Poecilia reticulata		n	S				22	25	7d	LC50	Mortality	35.00	3		IUCLID 2000: Könemann, 1981
Poecilia reticulata		y	R	GC std.			21		96h	LC50	Mortality	12.00	2	1, 3, 4	Galassi et al, 1998
Poecilia reticulata	2-3 months	n	R		tw		22	25	7d	LC50	Mortality	35.15	3	15	Könemann, 1981

Notes

1 According to OECD guidelines
2 Concentrations measured at beginning and end of test
3 Concentrations measured at renewals
4 Mean measured concentrations
5 Recalculated from mmol/m3
6 Artificial pond water
7 Photoperiod 12 hours
8 Recalculated from 0,26 mM
9 Recalculated from 4,08 log1/value (mol/l); 14h light, 10h dark
10 Recalculated from 0,06 mM
11 Recalculated from 0,09 mM
12 Water analysis 4x/day
13 Large differences in weight
14 All concentratrions are nominal
15 Recalculated from 2,52 uM
16 Recalculated from Log1/LC50 (mg/l)
17 Geomean of 17,2, 19,6 and 15,7

Table A2.5. Acute toxicity of o-xylene to marine organisms.

Species	Species properties	A	Test type	Purity [%]	Test water	pH	T [°C]	Salinity [‰]	Exp. time	Criterion	Test endpoint	Value [mg/l]	Validity	Notes	Reference
Bacteria															
Vibrio fischeri										EC50	Bioluminescence	9.25	2	1	Hermens et al, 1985
Vibrio fischeri		n	S		am		15	20	15m	EC20	Bioluminescence	16.67	3	7	Kafka et al, 1995
Vibrio fischeri			Sc	>95	dw		20	3% NaCl	15m	EC50	Luminescence	8.83	2	5	Zhao, 1995
Crustacea															
Artemia		y	Sc		aw	8.3-8.4	19.5-22	30	48h	LC50	Mortality	24.64	2	6	MacLean and Doe, 1989
Artemia		n	Sc	>97			20	30	24h	LC50	Mortality	23.67	3	2	Abernethy et al, 1986
Crago franciscorum	1.8g	y	S	>99	nw		16	25	96h	LC50	Mortality	1.30	3	3	Benville and Korn, 1977
Cancer magister dana	larvae	n	S				13	30	48h	LC50	Mortality	38.00	4		IUCLID 2000: Caldwell et al, 1977
Echinodermata															
Strongylocentrotus droebachiensis	eggs. first day after fertilisation	y	S	>98	nw				96h	EC50		4.10	2	4	Falk-Petersen et al, 1985
Pisces															
Morone saxatilis	6.0g	y	S	>99	nw		16	25	96h	LC50	Mortality	11.00	3	3	Benville and Korn, 1977

Notes

1 Microtox test
2 Methods in Wells et al 1982, value recalculated from mmol/m3
3 >99% loss of concentration after 96h, GC analysis after 0, 24, 48, 72, 96 hours
4 Beakers covered with aluminium foil, fluometrical analysis during experiment
5 Recalculated from log1/value (3,79 mol/l)
6 Geomean of 27,1 and 22,4
7 2% 2-propanol added

Table A2.6. Chronic toxicity of o-xylene to freshwater organisms.

Species	Species properties	A	Test type	Purity [%]	Test water	pH	T [°C]	Hardness [mg $CaCO_3$/l]	Exp. time	Criterion	Test endpoint	Value [mg/l]	Validity	Notes	Reference
Algae															
Pseudokirchneriella subcapitata		y	Sc			neutral			8d	NOEC	Growth	1	2	1	Herman et al, 1990
Chlorella vulgaris	30000 cells/ml	n	Sc		am		20		24h	EC10	Growth rate	12.47	3		Kauss and Hutchinson, 1975

Notes

1 16h-8h light-dark cycle, unclear when analysis is performed

Table A2.7. Acute toxicity of p-xylene to freshwater organisms.

Species	Species properties	A	Test type	Purity [%]	Test water	pH	T [°C]	Hardness [mg $CaCO_3$/l]	Exp. time	Criterion	Test endpoint	Value [mg/l]	Validity	Notes	Reference
Protozoa															
Tetrahymena pyriformis		n	S	>95	am	7.35	27		48h	IC50	Growth	88.10	3	1	Schultz et al, 1996
Algae															
Chlamydomonas sp.									3h	EC50	Inhib. photosyn.	45.70	4		IUCLID 2000: Hutchinson et al, 1980
Chlorella vulgaris		n							3h	EC50	Inhib. photosyn.	105.10	4		IUCLID 2000: Hutchinson et al, 1980
Pseudokirchneriella subcapitata		y	Sc?	GC std					72h	EC50	Growth	3.20	2	2, 3, 5	Galassi et al, 1998
Pseudokirchneriella subcapitata	10E3 cells/ml	y	Sc	>99	am	7.8-7.9	22.2	24.2	73h	EC50	Growth	4.36	1		
Scenedesmus quadricauda		y	S	GC standard	am	7.5	22		96h	EC50	Growth	9.56	2	3, 10	Di Marzio and Saenz, 2006
Crustacea															
Daphnia magna	24h	y	Sc		am	7.4-7.9	20.5-21	250	48h	LC50	Mortality	32.24	2	15	MacLean and Doe, 1989
Daphnia magna	4 - 6 days	n	Sc	>97	dw	6.5	23		48h	LC50	Mortality	8.49	2	6	Bobra et al, 1983
Daphnia magna			Sc	GC std					24	IC50	Immobilisation	3.60	2	2, 3, 5	Galassi et al, 1998
Daphnia magna	6-24h old		Sc	>95	dw		22		24h	IC50	Immobilisation	22.18	2	11	Zhao, 1995
Daphnia spinulata	< 24h	y	S	GC std	am	7.8	20	95.8	48h	LC50	Mortality	4.25	2	3, 7, 8	Di Marzio and Saenz, 2006

Species	Species properties	A	Test type	Purity [%]	Test water	pH	T [°C]	Hardness [mg $CaCO_3$/l]	Exp. time	Criterion	Test endpoint	Value [mg/l]	Validity	Notes	Reference
Hyalella curvispina	10 day	y	S	GC std	dw	8.3	21	82	96h	LC50	Mortality	4.25	2	3, 8	Di Marzio and Saenz, 2006
Rotifera															
Brachionus calyciflorus			S		rw	7.5	25		24h	LC50	Mortality	253.00	3	13	Juchelka and Snell, 1994
Pisces															
Bryconamericus iheringii	4.7 cm. 2.85g	y	Sc	GC std	am	7.9	20	98	96h	LC50	Mortality	6.37	1	2, 3, 5, 9	Di Marzio and Saenz, 2006
Bryconamericus iheringii	2.85g. 4.7cm	y	Sc	GC std					96h	LC50	Mortality	6.90	2	2, 3, 5	Di Marzio and Saenz, 2004
Carassius auratus	6.2 cm. 3.3 g	y	S		tw	6-7	20		24h	LC50	Mortality	18.00	3	1, 3	Bridie et al, 1979
Cnesterodon decemmaculatus		y	Sc	GC std	dw	8.59	19.5	141.6	96h	LC50	Mortality	6.17	2	2, 3, 4, 14	Di Marzio et al, 2001
Oncorhynchus mykiss		y	R	GC std			12		96h	LC50	Mortality	2.60	2	2, 4, 5	Galassi et al, 1998
Pimephales promelas		y	Sc	GC std					96h	LC50	Mortality	8.91	2	2, 3, 5	Di Marzio and Saenz, 2001
Poecilia reticulata		y	R	GC std			21		96h	LC50	Mortality	8.80	2	2, 4, 5	Galassi et al, 1998
Poecilia reticulata	2-3 mo	n	R		tw		22	25	7d	LC50	Mortality	35.15	3	12	Könemann, 1981

Notes

1	System not closed, no prevention of volatilisation
2	According to OECD guidelines
3	Concentrations measured at beginning and end of test
4	Concentrations measured at renewals
5	Mean measured concentrations
6	Recalculated from mmol/m^3
7	Artificial pond water
8	Recalculated from 0,04 mM
9	Recalculated from 0,06 mM
10	Recalculated from 0,09 mM
11	Recalculated from 0,09 mM
12	Recalculated from 2,52 uM
13	Value exceeds water solubility
14	Recalculated from Log1/LC50 (mg/L)
15	Geomean of 37, 31,5, 33,1 and 28

Table A2.8. Acute toxicity of p-xylene to marine organisms.

Species	Species properties	A	Test type	Purity	Test water	pH	T [°C]	Salinity [‰]	Exp. time	Criterion	Test endpoint	Value [mg/l]	Validity	Notes	Reference
Bacteria															
Vibrio fischeri			Sc	>95	dw		20	3% NaCl	15m	EC50	Luminescence	17.22	2	3	Zhao, 1995
Crustacea															
Artemia		y	Sc		aw	8.1-8.2	21-22.5	30	24h	LC50	Mortality	27.80	2		MacLean and Doe, 1989
Artemia		n	Sc	>97			20	30	24h	LC50	Mortality	24.63	3	1	Abernethy et al, 1986
Crago franciscorum	1.8g	y	S	>99	nw		16	25	96h	LC50	Mortality	2.00	3	2	Benville and Korn, 1977
Pisces															
Morone saxatilis	6.0g	y	S	>99	nw		16	25	96h	LC50	Mortality	2.00	3	2	Benville and Korn, 1977

Notes

1	Methods in Wells et al 1982, value recalculated from mmol/m3
2	>99% loss of concentration after 96h, GC analysis after 0, 24, 48, 72, 96 hours
3	Recalculated from log1/value (4,08 mol/l)

Table A2.9. Chronic toxicity of p-xylene to freshwater organisms.

Species	Species properties	A	Test type	Purity [%]	Test water	pH	T [°C]	Hardness [mg $CaCO_3$/l]	Exp. time	Criterion	Test endpoint	Value [mg/l]	Validity	Notes	Reference
Algae															
Pseudokirchneriella subcapitata		y	Sc			neutral			8d	NOEC	Growth	0.9	1		Herman et al, 1990
Pseudokirchneriella subcapitata	CCAP 278/4, 10E3 cells/ml	y	Sc	>99	am	7.8-7.9	22.2	24.2	73h	NOEC	Growth	0.44	1	1	Oldersma et al 2004 (TNO Report)
Pseudokirchneriella subcapitata	CCAP 278/4, 10E3 cells/ml	y	Sc	>99	am	7.8-7.9	22.2	24.2	73h	EC10	Growth	1.90	1	1	Oldersma et al 2004 (TNO Report)

Notes

1 OECD, GLP

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