National Institute for Public Health
and the Environment
Ministry of Health, Welfare and Sport

Environmental risk limits for xylenes

Update of the 2009 report

RIVM Letter report 2014-0043

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Het RIVM doet voorstellen voor nieuwe risicogrenzen voor de stof xyleen in water, bodem en lucht. Aanpassing was nodig omdat er aanvullende gegevens beschikbaar waren en omdat de Europese methodiek om waterkwaliteitsnormen af te leiden, is veranderd.

Xyleen wordt gebruikt in brandstof voor motoren en als grondstof voor de productie van polyesterverbindingen. De stof komt voor in drie verschillende vormen (isomeren), die elk een iets andere chemische structuur hebben: ortho-, meta- en para-xyleen. Omdat de giftigheid van deze afzonderlijke isomeren van xyleen vergelijkbaar is, worden ze in dit rapport als een groep behandeld. Om te bepalen of de risicogrenzen worden overschreden, moeten daarom de meetgegevens van alle drie de isomeren bij elkaar worden opgeteld. Op basis van deze totale hoeveelheid kan een conclusie worden getrokken.

De voorgestelde normen voor oppervlaktewater zijn inmiddels overgenomen door het ministerie van Infrastructuur en Milieu.

Trefwoorden: xylenen, waterkwaliteitsnormen, risicogrenzen

Abstract

RIVM proposes new risk limits for xylene xyleen in water, soil and air. Revision was needed because additional data have become available and because of changes in the European methodology for deriving water quality standards.

Xylene is used in engine fuels and as a basis for the production of polyester. The chemical exists in three different chemical forms (isomers), each of which has a slightly different chemical structure: ortho-, meta- and para-xylene. Because these isomers have comparable ecotoxicity, they are considered as a group in this report. The summed concentrations of the three isomers should be used to draw conclusions on compliance of monitoring data with the standards.

The proposed quality standards for surface water have been adopted by the Ministry of Infrastructure and the Environment.

Keywords: xylenes, water quality standards, risk limits

Contents

Summary

In this report, updated environmental risk limits (ERLs) for surface water (freshwater and marine), soil, groundwater and air are derived for xylenes. Xylenes are listed as a specific pollutant in the Dutch decree on monitoring in the context of the Water Framework Directive (WFD). An update of the existing water quality standards was considered necessary because additional chronic ecotoxicity data have become available, which allow for a lower assessment factor than used previously. Changes in the methodology for deriving water quality standards under the WFD were implemented as well. The proposed standards for surface water have been adopted by the Ministry of Infrastructure and the Environment and will be used for the preparation of the next generation of river basin management plans under the WFD.

Xylene can be present in three forms: the isomers ortho-, meta- and paraxylene. Based on an analysis of ecotoxicity data for the individual isomers, it is concluded that effect levels are similar. The differences between the previously derived standards for the individual isomers were due to the different datasets rather than to differences in ecotoxicity. Therefore, the isomers are treated as a group in this report and the proposed ERLs apply to the isomers together.

The WFD-standards for surface water quality include the Annual Average EQS (AA-EQS) for long-term exposure and the Maximum Acceptable Concentration EQS (MAC-EQS) for short-term concentration peaks. A separate human-health based quality standard is derived for surface water that is used for drinking water abstraction ($QS_{dw, hh}$). Next to these WFD-specific standards, Maximum Permissible Concentrations (MPC) are derived for soil, groundwater and air, partly based on the aquatic dataset. For all compartments, the national specific risk limits Negligible Concentration (NC) and Serious Risk Concentration for ecosystems (SRC) are derived in addition. The derived risk limits are summarised in the table below:

Table 1 Derived AA-EQS, MAC-EQS, $QS_{dw, hh}$, MPC, NC, and SRC values for xylene. Values for water are given in two significant digits where appropriate.

Compartment	**Environmental Risk Limit**			
	AA-EQS	**MAC-EQS**	**NC**	**SRC**
Freshwater [µg/L]	17	244	0.17	872
Marine water [µg/L]	1.7	49	0.020	872
Surface water [µg/L] (drinking water abstraction)	500			
	MPC		**NC**	**SRC**
Soil [µg/kg dwt]	229	-	2.3	11600
Groundwater [µg/L]	17	-	0.17	872
Air [µg/m^3]	870	-	8.7	-

- = not applicable

1 Introduction

1.1 Reasons for the update

In this report, updated environmental risk limits (ERLs) for surface water (freshwater and marine), soil, groundwater and air are derived for xylenes. Xylenes are listed as a specific pollutant in the Dutch decree on WFD-monitoring (*Regeling monitoring Kaderrichtlijn water*). The current water quality standards are based on an RIVM report that was published in 2009 [1]. An update of that report was considered necessary for several reasons:

- The current chronic standards for water (2.44 and 0.24 µg/L for fresh and saltwater, respectively) were derived by applying a high assessment factor on the acute ecotoxicity data, because chronic ecotoxicity data were present for algae only. Meanwhile it was noted that valid ecotoxicity studies for crustaceans have become available.
- Since the publication of the 2009-report, the guidance for deriving water quality standards under the Water Framework Directive (WFD) has been updated [2]. According to the new guidance, a lower assessment factor may be applied when deriving the risk limit for peak exposure of non-bioaccumulating substances in water.
- In the 2009-report, separate ERLs were derived for the individual isomers, and for the xylenes as a group, while it was noted that the latter was most appropriate. The large differences in ERLs for the individual isomers were merely the result of differences in the datasets which led to different assessment factors. Because there is no need to present ERLs for the individual isomers, they are left out in this report.
- In the 2009-report, a provisional drinking water standard was used to derive a quality standard for surface water intended for drinking water abstraction. According to the WFD-guidance, the WHO guidelines for drinking water quality should be used.

1.2 Environmental risk limits in the Netherlands

Three types of ERLs are considered in the Dutch policy on substances: the Maximum Permissible Concentration (MPC), the Negligible Concentration (NC) and the Serious Risk Concentration (SRC). These ERLs are denoted as *Maximaal Toelaatbaar Risiconiveau (MTR)*, *Verwaarloosbaar Risiconiveau (VR) and Ernstig Risiconiveau (ER)*, respectively, and are described as follows:

- Maximum Permissible Concentration (MPC) – defined in [3,4] as the standard based on scientific data which indicates the concentration in an environmental compartment for 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} per year of death can be calculated (for carcinogenic substances).

- Negligible Concentration (NC) – the environmental concentration at which effects to ecosystems are expected to be negligible and functional properties of ecosystems are safeguarded fully. It defines a safety margin which should exclude combination toxicity. The NC is derived by dividing the MPC by a factor of 100.

- Serious Risk Concentration for ecosystems (SRC_{eco}) – the environmental concentration at which possibly serious ecotoxicological effects are to be expected. The SRC_{eco} for water is valid for the freshwater and saltwater compartment.

With the implementation of the WFD, the MPC for fresh- and marine surface water has been replaced with two quality standards to cover both long- and short-term effects resulting from exposure:

- a long-term standard, indicated as the annual average environmental quality standard (AA-EQS) and normally based on chronic toxicity data, and
- a short-term standard, referred to as a maximum acceptable concentration EQS (MAC-EQS) which is based on acute toxicity data.

The terms AA-EQS and MAC-EQS are used in the European priority substances directive 2013/39/EU[1] and are indicated as 'JG-MKN' and 'MAC-MKN', respectively[2], in Dutch legislation based on the WFD. In addition, a quality standard for surface water intended for drinking water extraction is derived ($QS_{dw, hh}$). The WFD-standards are described as follows:

- Annual Average EQS (AA-EQS) – a long-term standard, expressed as an annual average concentration (AA-EQS) and normally based on chronic toxicity data which should protect the ecosystem agains adverse effects resulting from long-term exposure.

  The AA-EQS should not result in risks due to secondary poisoning and/or risks for human health aspects. These aspects are therefore also addressed in the AA-EQS, when triggered by the characteristics of the compound (i.e. human toxicology and/or potential to bioaccumulate). Separate AA-EQSs are derived for the freshwater and saltwater environment.

- Maximum Acceptable Concentration EQS (MAC-EQS) for aquatic ecosystems – the concentration protecting aquatic ecosystems from effects due to short-term exposure or concentration peaks. The MAC-EQS is derived for freshwater and saltwater ecosystems, and is based on direct ecotoxicity only.

- Quality standard for surface water that is used for drinking water abstraction ($QS_{dw, hh}$). This is the concentration in surface water that meets the requirements for use of surface water for drinking water production. The $QS_{dw, hh}$ specifically refers to locations that are used for drinking water abstraction.

The quality standards for water in the context of the WFD refer to the absence of any impact on community structure of aquatic ecosystems. Hence, long-term undisturbed function is the protection objective under the WFD, not the potential to recover after transient exposure.

[1] Directive 2013/39/EU of the European Parliament and of the Council of 12 August 2013 amending Directives 2000/60/EC and 2008/105/EC as regards priority substances in the field of water policy.
[2] JG = Jaargemiddelde = annual average; MKN = milieukwaliteitsnorm = environmental quality standard.

Given the methodology and protection goals, the definition of the AA-EQS more or less equals that of the former MPC for water. However, the risk for predators due to secondary poisoning, and exposure of humans via fish consumption have now explicitly been integrated in the AA-EQS. For genotoxic substances, the WFD uses cancer probability of 10^{-6} *per life* in line with the recommendations in the REACH-guidance [2,5]. As indicated above, the Dutch MPC is related to instead of 10^{-6} *per year*, which considered equal to 10^{-4} per life. Furthermore, the MPC used to be compared with 90^{th} percentile of the measured concentrations, while under the WFD the annual average concentration is used for complicance checking.

Table 2 gives a summary of the risk limits used in Dutch environmental protection policy.

*Table 2 Types of risk limits and exposure routes considered for the respective compartments. Compartments/routes indicated with * are subject of trigger values: derivation of risk limits depends on the characteristics of the compound.*

Compartment	Type of risk limit	Route considered
air	MPC NC	humans via inhalation
soil	MPC NC	humans via consumption of vegetables, meat, milk* predatory birds / mammals via earthworms* soil organisms
	SRC	soil organisms
groundwater	MPC NC	humans via drinking water groundwater organisms
	SRC	groundwater organisms
sediment*	MPC NC SRC	sediment organisms
water	AA-EQS NC	humans via fish consumption* predatory birds / mammals via fish* water organisms
	MAC-EQS SRC	water organisms
	$QS_{dw, hh}$	humans via drinking water

MPC = Maximum Permissible Concentration
NC = Negligible Concentration
SRC = Serious Risk Concentration
EQS = Environmental Quality Standard
AA-EQS = Annual Average EQS
MAC-EQS = Maximum Acceptable Concentration EQS
$QS_{dw, hh}$ = Quality Standard for surface water intended for drinking water abstraction

1.3 Risk limits or quality standards

In the Netherlands, there has always been a clear distinction between scientifically based advisory values, indicated as environmental *risk limits*, and the final regulatory values, indicated as environmental *quality standards*. Standards are set by the responsible ministeries primarily on the basis of a scientific advice, but other (socio-economic) aspects may be taken into account as well. It may happen that the final standard deviates from the scientifically based risk limit. Therefore, the national guidance documents and reports based thereon refer as much as possible to the derivation of *risk limits*, the word *standard* is preferably not used to avoid the suggestion that this policy step has already been taken. However, special considerations are made for the water compartment. As indicated above, compliance check differs between the WFD water quality standards and the previously used MPC (*MTR*) values. To prevent confusion, the abbreviations MPC (and *MTR*) have been abandoned for the water compartment and the terminology of the WFD-guidance is followed instead. Still, although indicated as quality standards (EQS), the values that are derived in this report should be interpreted as being risk limits, in a sense that they are scientific advisory values until approved as official standards by the responsible ministry.

1.4 Methodology

1.4.1 Water and sediment

The methodology for the derivation of quality standards for water and sediment is laid down in the European guidance document for derivation of environmental quality standards under the WFD [2]. This document is further referred to as the WFD-guidance. Due to the characteristics of xylenes, derivation of risk limits for sediment is not considered relevant according to the triggers of the WFD-guidance. Additional guidance for derivation of ERLs that are specific for the Netherlands, such as the NC and SRC, can be found in [6], further referred to as the INS-guidance. Similar to the WFD-guidance, the INS-guidance is based on the Technical Guidance Document (TGD), issued by the European Commission and developed in support of the risk assessment of new notified chemical substances, existing substances and biocides [7] and on the Manual for the derivation of Environmental Quality Standards in accordance with the Water Framework Directive [8]. The WFD-guidance also takes into account the most recent guidance developed under REACH [5].

1.4.2 Soil, groundwater and air

For derivation of ERLs for soil, groundwater and air, the INS-guidance is followed. As for water, the guidance for these other environmental compartments builds on the Technical Guidance Document (TGD), issued by the European Commission and developed in support of the risk assessment of new notified chemical substances, existing substances and biocides [7].

1.4.3 Data sources

For the 2009-report, 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 addition to this, all references in the RIVM e-tox base and US EPA ECOTOX database were evaluated (an additional 30 references).

For the current report, an additional on-line literature search was performed via SCOPUS, available via http://www.scopus.com/ in December, 2013. For information on coverage, see http://info.scopus.com/detail/what/. This search did not result in additional references from which an endpoint could be derived, neither did the US EPA database contain new studies. The public REACH summary dossiers for o-, m-, and p-xylene were consulted via the ECHA website (www.echa.europe.eu) and additional data for crustaceans and algae were retrieved.

1.4.4 *Data evaluation*

For the 2009-report, ecotoxicity studies were screened for relevant endpoints (i.e. those endpoints that have consequences at the population level of the test species) and thoroughly evaluated with respect to the validity (scientific reliability) of the study. A detailed description of the evaluation procedure is given in the Annex to the EQS-guidance under the WFD. In short, the following reliability indices were assigned, based on [9]:

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.).'

Citations
In case of (self-)citations, the original (or first cited) value is considered for further assessment, and an asterisk is added to the Ri of the endpoint that is cited.

The data of the 2009-report were used in this report without additional re-evaluation. The available studies are 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.

1.4.5 *Data treatment*

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).

For the xylene isomers, fast volatilisation puts 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.

After data collection and validation, toxicity data were combined into an aggregated data table with one effect value per species according to the 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. Geometric means were calculated with unrounded figures, the aggregated data are presented in three digits where underlying data allow, otherwise in two.

1.5 Status of the results

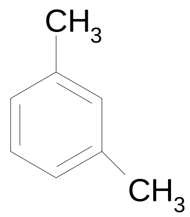
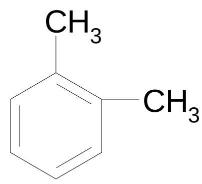
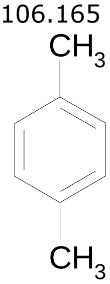
The results presented in this report have been discussed by the members of the scientific advisory group for standard setting in the Netherlands (*Wetenschappelijke Klankbordgroep normstelling water en lucht*). As indicated above, the ERLs in this report are scientifically derived values, based on (eco)toxicological, fate and physico-chemical data. They serve as advisory values for the Dutch Steering Committee for standard setting for water and air, which is appointed to set the final standards.

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

2.1 Identity and use of m-, o- and p-xylene

The identity of the xylene isomers is presented in Table 3.

Table 3 Identity of m-, o-, and p-xylene. Data from [10]

Parameter	Name or number
Chemical name	1,3-dimethylbenzene
Common/trivial/other name	meta-xylene, m-xylol, 3-methyltoluene
CAS number	108-38-3
EC number	203-576-3
Molecular weight	106.165
Structural formula	
SMILES code	Cc1cccc(C)c1
Chemical name	1,2-dimethylbenzene
Common/trivial/other name	ortho-xylene, o-xylol, 2-methyltoluene
CAS number	95-47-6
EC number	202-422-2
Molecular weight	106.165
Structural formula	
SMILES code	Cc1ccccc1C
Chemical name	1,4-dimethylbenzene
Common/trivial/other name	para-xylene, p-xylol, 4-methyltoluene
CAS number	106-42-3
EC number	203-396-5
Molecular weight	106.165
Structural formula	
SMILES code	Cc1ccc(C)cc1

The following information on production and use is obtained from [11]:
A large proportion of xylenes is used in motor fuel, due to gasoline containing about 10% xylenes. The capacity for production of pure xylene was 35,000,000 tonnes in Asia, the USA and the EU in 2010. The main part is used for further separation in the three isomers through distillation fractionated crystallisation. 82 % ends up in p-xylene for the production of phtalate compounds that are used for polyester, e.g. polyethylene terephthalate (PET). About 10% ends up as o-xylene used for synthesis of phthalic acid anhydride to polymers and phthalates, and about 1 % becomes meta-xylene for isophthalic acid. All three isomers are raw materials for synthesis of special chemicals such as vitamins, pharmaceuticals, flavouring agents etc. About 10 % of the world production, is estimated to be used as the isomer mixture xylene. It is used as a solvent in a number of products where good solvent capacity and relatively fast evaporation are needed, such as paints, degreasing agents, glues, sealing agents and carcare products.

2.2 Physico-chemical properties

The physico-chemical properties of the xylene isomers are summarised in the tables below. Data originate from [10].

Table 4 Physico-chemical properties of m-xylene.

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

Table 5 Physico-chemical properties of o-xylene.

Parameter	**Unit**	**Value**	**Remark**
Water solubility	[mg/L]	240	20°C, shake flask
log K_{OW}	[-]	3.12	
log K_{OC}	[-]	2.35	organic carbon ≥ 4.02%, batch-equilibrium, GC
Vapour pressure	[Pa]	767	20°C
		987	30°C
		6354	63.5°C
Melting point	[°C]	-25.2	
Boiling point	[°C]	144.5	
Henry's law constant	[Pa.m^3/mol]	594	20°C, EPICS-GC

Table 6 Physico-chemical properties of p-xylene.

Parameter	Unit	Value	Remark
Water solubility	[mg/L]	191	20°C, shake flask
log K_{OW}	[-]	3.15	
log K_{OC}	[-]	2.37	HPLC screening method
Vapour pressure	[Pa]	787	20°C
Melting point	[°C]	13.25	
Boiling point	[°C]	138.37	
Henry's law constant	[Pa.m^3/mol]	754	EPIC-GC-FID

2.3 Behaviour in the environment

Xylenes are not susceptible to hydrolysis [10]. Photolysis half-life is 9.6 hours for m-xylene and 30 hours for o-xylene [12]. In water, volatilisation seems to be the dominant removal process [10], with half-lives of about 3 hours at 1 m depth, wind speed 3 m/s, current 1 m/s.

2.4 Bioconcentration

An overview of the bioaccumulation data for xylenes is given in Table 7. Detailed bioaccumulation data are tabulated in Appendix 1. Based on these BCF-values, a default biomagnification factor (BMF) of 1 is assumed.

Table 7 Overview of bioaccumulation data for xylenes.

Substance	BCF [L/kg]	Remark	Reference
m-xylene	6.43	molluscs	[13]
	23	fish; exposure in crude oil suspension	[10,14]
o-xylene	7.25	molluscs	[13]
	21.4	fish; exposure in crude oil suspension	[14]
p-xylene	23.6	fish; exposure in crude oil suspension	[14]

2.5 Human toxicology

The Tolerable Daily Intake (TDI) for xylenes is 150 µg/kg bw day [15]. Harmonised classification of the respective xylenes with respect to human toxicology under the CLP Regulation 1272/2008/EC is as follows: H312 (harmful in contact with skin), H315 (causes skin irritation), H332 (harmful if inhaled). The xylene isomers are included in the Community Rolling Action Plan under REACH [16], because of concerns about a.o. suspected carcinogenic, mutagenic or reprotoxic (CMR) properties. The substance evaluation, which will be carried out by Germany, is scheduled for 2015[3] and may eventually lead to an adapted classification.

2.6 Trigger values

The collected properties for m-, o-, and p-xylene are compared to the triggers for ERL-derivation according to the WFD-guidance.

[3] http://echa.europa.eu/information-on-chemicals/evaluation/community-rolling-action-plan/

Table 8 Collected properties for comparison to ERL triggers.

Parameter	**m-xylene**	**o-xylene**	**p-xylene**	**Reference**
log $K_{p,susp-water}$ [log L/kg][a]	1.33	1.35	1.37	see 2.2
BCF [L/kg]	23	21.4	23.6	see 2.4
BMF		1		see 2.4
log K_{OW}	3.15	3.12	3.15	see 2.2
R-phrases		H312, H315, H332		see 2.5
A1 value		not available		
WHO drinking water standard		500 µg/L		[17]

a: $K_{OC} \times f_{OC,susp}$; $f_{OC,susp}$ = 0.1 kg_{OC}/kg_{solid} [2,7]

Since the log $K_{p,susp-water}$ is < 3, derivation of the MPC for sediment is not triggered and expression of the quality standards for water on the basis of suspended matter is not needed. The BCF is < 100 L/kg, assessment of secondary poisoning is not needed.

Derivation of the water quality standard for human consumption of fish is not triggered based on the current classification, but possible future classification as CMR would trigger such a derivation. However, based on the TDI and the reported BCF, the outcome would not be critical as compared to the derived values based on ecotoxicity (see section 3.3). Therefore, this route is not further evaluated.

3 Toxicity data and derivation of risk limits for water

3.1 Differences between isomers

The available ecotoxicity data are presented in Appendix 2. The dataset for marine species is too small for a meaningful comparison. There are no further indications of a difference in sensitivity between freshwater and marine organisms. Therefore, the fresh- and saltwater data are combined into one dataset. Very view valid chronic data are available, and a comparison between the respective isomers can only be made on the basis of the acute data. Table 9 shows the individual acute data for the most sensitive endpoint per species.

Table 9. Overview of valid acute ecotoxicity data for xylene isomers. Marine species are indicated with (sw). Data are rounded to three significant digits where underlying data allow, otherwise to two.

Taxon/	**L(E)C50 [mg/L]**		
Species	**m-xylene**	**o-xylene**	**p-xylene**
Bacteria			
Vibrio fischeri (sw)	19.3	8.83, 9.25	17.2
Algae			
Pseudokirchneriella subcapitata		4.70	3.20, 4.36
Scenedesmus quadricauda	7.43	27.6	9.56
Crustacea			
Artemia salina (sw)[a]	7.85	11.7	18.4
Ceriodaphnia cf. dubia	2.44		
Daphnia magna [b]	4.70, 23.8	1.00, 17.2	3.60, 22.2
Daphnia spinulata	4.25	6.37	4.25
Hyalella curvispina	4.25	6.37	4.25
Pisces			
Bryconamericus iheringii	11.7, 11.2	9.56, 9.94	6.37, 6.90
Carassius auratus [c]		16.1	
Cataostomus commersoni		16.1	
Cnesterodon decemmaculatus	10.7	9.33	6.17
Lepomis macrochirus		16.1	
Oncorhynchus mykiss [d]	8.40	7.60	2.60
Oryzias latipes	32.0		
Pimephales promelas [d]	15.5	16.2	8.91, 4.70
Poecilia reticulata	12.9	12.0	8.80
Echinodermata			
Strongylocentrotus droebachiensis (sw)		4.10	

a: 48-hours immobilisation
b: 24-hours immobilisation
c: endpoint for relevant test duration (48 hours) included only
d: data for 96 hours selected

Using ANOVA (with unrounded data), there is no significant difference between the datasets for the three isomers. To compare the toxicity of the isomers, species sensitivity distributions (SSD) were made with ETX 2.0 [18], using the unrounded data for all xylenes together, or the separate data for the individual isomers. Note that these SSDs are made only for the purpose of comparing the datasets, and not for derivation of ERLs. Table 10 shows the results of the SSD calculations.

Table 10. Characteristics of the Species Sensitivity Distributions (SSDs) constructed using the unrounded data for all xylenes, and for the m-, o- and p-isomer.

	Parameters of the normal distribution			
	all xylenes	**m-xylene**	**o-xylene**	**p-xylene**
mean	0.92	0.97	0.96	0.82
standard deviation	0.30	0.31	0.31	0.28
number of data	50	15	19	16
	HC5 results [mg/L]			
	all xylenes	**m-xylene**	**o-xylene**	**p-xylene**
HC5	2.64	2.88	2.75	2.27
lower limit	1.99	1.54	1.60	1.32
upper limit	3.32	4.30	3.97	3.24
spread	1.67	2.79	2.48	2.45
HC50	8.36	9.44	9.17	6.68
lower limit	7.09	6.84	6.89	5.04
upper limit	9.86	13.01	12.22	8.86
spread	1.39	1.90	1.77	1.76

Figure 1 shows the respective SSD-curves. As can be seen from the data in Table 10 and Figure 1, the SSD-results for the combined xylenes are similar to that of o- and m-xylene. The curves for o- and m-xylene are at the right hand side, indicating that the sensitivity towards these isomers is generally lower as compared to p-xylene. However, the lower tail of the distribution of the combined xylenes is determined by the low values for *Ceriodaphnia dubia* and *Daphnia magna* obtained with o-xylene.

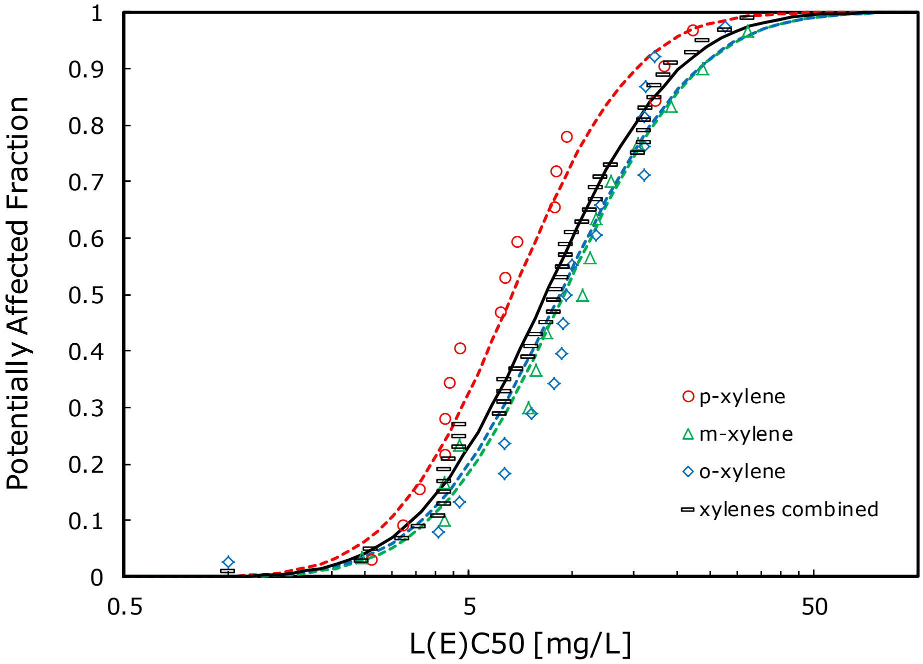


Figure 1. Species Sensitivity Distributions based on acute endpoints for all xylenes, and for the m-, o- and p-isomer. The X-axis represents acute L(E)50-values in mg/L, presented on a log-scale. The Y-axis represents the potentially affected fraction.

Figure 2 and 3 show the median estimates of the HC5 and HC50, respectively, with upper and lower limits. The HC5 for m-xylene is higher than the other values, but has a larger 95% confidence interval. The confidence intervals around the respective HC5-values overlap. The difference between the HC5 for all xylenes and the lowest HC5 for p-xylene is a factor of 1.2. The HC50-values of m-, o- and p-xylene are also ranked in decreasing order, but the difference between the highest HC50 for m-xylene and the lowest for p-xylene is relatively small (factor of 1.4). The difference between all xylenes and p-xylene is a factor of 1.3. The 95% confidence limits still overlap. Based on this analysis, it is considered justified to group the data and use them to derive a single value per species for xylene (Table 11).

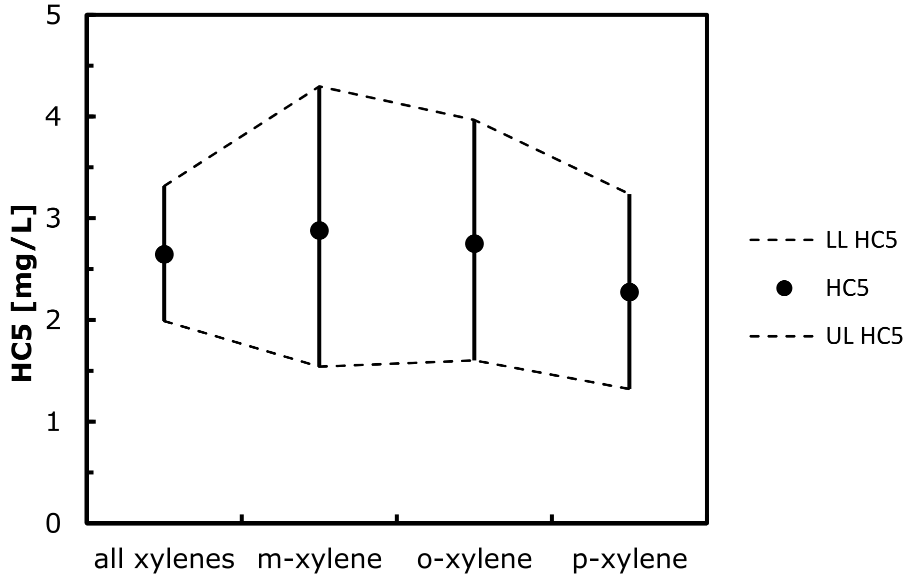


Figure 2. Estimates of the HC5 and lower and upper limits (LL, UL) based on acute L(E)50-values for all xylenes, and for the m-, o- and p-isomer.

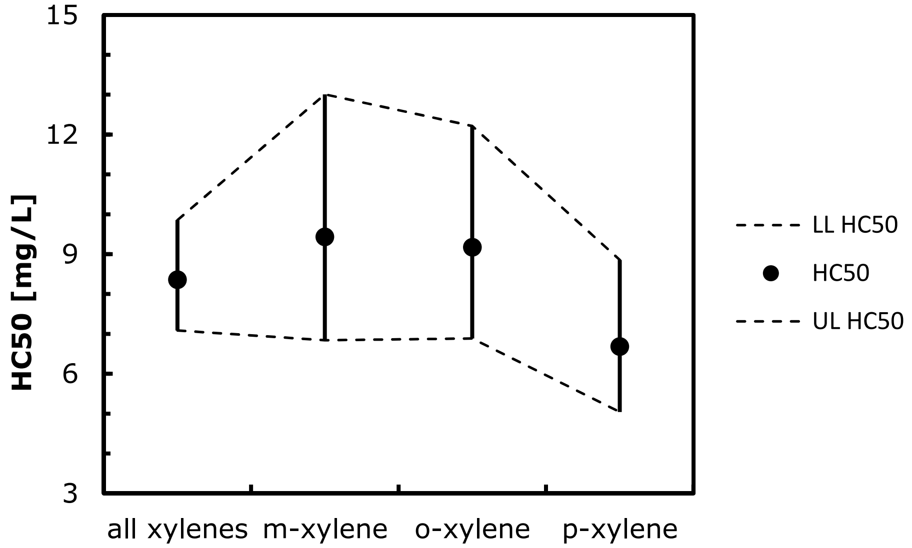


Figure 3. Estimates of the HC50 and lower and upper limits (LL, UL) based on acute L(E)50-values for all xylenes, and for the m-, o- and p-isomer.

Table 11. Xylene: selected aquatic toxicity data for ERL derivation. Values represent lowest endpoint per species, test results from individual isomers are indicated in footnotes by (m), (o) or (p) for m-, o-, or p-xylene, respectively. See also Table 5. Marine species are indicated with (sw). Geometric means are calculated with unrounded values and expressed in three significant digits where underlying data allow, otherwise in two.

Acute Taxonomic group/ *species*	**L(E)C50 [mg/L]**	**Chronic** Taxonomic group/ *species*	**NOEC [mg/L]**
Bacteria			
Vibrio fischeri (sw)	12.8[a]		
Algae		**Algae**	
Pseudokirchneriella subcapitata	4.03[b]	*Pseudokirchneriella subcapitata*	0.86[o]
Scenedesmus quadricauda	12.5[c]		
Crustacea		**Crustacea**	
Artemia salinia (sw)	11.9[d]	*Ceriodaphnia dubia*	1.2[e]
Ceriodaphnia cf. dubia	2.44[e]	*Daphnia magna*	1.57[p]
Daphnia magna	7.32[f]		
Daphnia spinulata	4.86[g]		
Hyalella curvispina	4.86[g]		
Pisces			
Bryconamericus iheringii	9.04[h]		
Carassius auratus	16.1[i]		
Cataostomus commersoni	16.1[i]		
Cnesterodon decemmaculatus	8.51[j]		
Lepomis macrochirus	16.1[i]		
Oncorhynchus mykiss	5.50[k]		
Oryzias latipes	32.0[e]		
Pimephales promelas	10.1[l]		
Poecilia reticulata	11.1[m]		
Echinodermata			
Strongylocentrotus droebachiensis (sw)	4.1[n]		

a geometric mean of 19.3 (m), 8.83 (o), 9.25 (o), 17.2 (p)
b geometric mean of 4.7 (o), 3.2 (p), 4.36 (p)
c geometric mean of 7.43 (m), 27.6 (o), 9.56 (p)
d geometric mean of 7.85 (m), 11.7 (o), 18.4 (p)
e one value available (m)
f geometric mean of 4.7 (m), 23.8 (m), 1 (o), 17.2 (o), 3.6 (p), 22.2 (p), 24-hours immobilisation
g geometric mean of 4.25 (m), 6.37 (o) and 4.25 (p)
h geometric mean of 11.7 (m), 11.2 (m), 9.56 (o), 9.94 (o), 6.37 (p) and 6.9 (p)
i one value available (o) for most relevant test duration (48 hours)
j geometric mean of 10.7 (m), 9.33 (o) and 6.17 (p)
k geometric mean of 8.40 (m), 7.60 (o) and 2.60 (p), 96-hours LC50
l geometric mean of 15.5 (m), 16.2 (o), 8.91 (p) and 4.7 (p), 96-hours LC50
m geometric mean of 12.9 (m), 12.0 (o) and 8.80 (p)
n one value available (o)
o geometric mean of 0.7 (m), 1 (o) and 0.9 (p), 8-days NOEC
p one value available (p)

3.2 Derivation of the MAC-EQS

3.2.1 Freshwater

The acute base set for xylene is complete, and the standard deviation of the log-transformed L(E)50-values is < 0.5. Therefore, an assessment factor of 10 can be used on the lowest EC50 value of 2.4 mg/L for *Ceriodaphnia cf. dubia.* This results in a MAC-EQS_{fw} of 2.44 / 10 = 0.244 mg/L = 244 µg/L.

3.2.2 Saltwater

There is one endpoint for a specific marine species (echinoderm), and the MAC-EQS_{sw} can be derived by putting an additional assessment factor of 5 on the MAC-EQS_{fw}. The MAC-EQS_{sw} is 48.8 µg/L.

3.3 Derivation of AA-EQS

Since secondary poisoning and human consumption of fish are not relevant for derivation of the AA-EQS, only the $QS_{fw, eco}$ and $QS_{sw, eco}$ for direct ecotoxicity are derived.

3.3.1 Freshwater

The acute base set is complete, chronic NOECs are available for algae and crustacea and the acutely most sensitive species is represented in the chronic dataset. Therefore, to derive the $QS_{fw, eco}$ an assessment factor of 50 is used on the lowest NOEC-value of 0.86 mg/L for *Pseudokirchneriella subcapitata*. This results in an AA-EQS_{fw} of 0.86 / 50 = 0.0172 mg/L = 17.2 µg/L.

3.3.2 Saltwater

The datasets for freshwater and marine species can be combined, but there is no chronic NOEC for a typically marine species. The $QS_{sw, eco}$ is therefore derived using an additional assessment factor of 10 on the $QS_{fw, eco}$. The AA-EQS_{sw} is 1.72 µg/L.

3.4 Derivation of the $QS_{dw, hh}$

For xylene, a drinking water standard of 500 µg/L is available [17]. According to the WFD, a substance specific removal rate should be considered to derive the $QS_{dw, hh}$. At present, such information is not available and water treatment is not taken into account. The $QS_{dw, hh}$ is 500 µg/L. It should be noted that concentrations of the substance at or below this health-based guideline value may affect the appearance, taste or odour of the water, leading to consumer complaints [17].

3.5 Derivation of the NC

The Negligible Concentration (NC) is derived by dividing the AA-EQS by a factor of 100, resulting in an NC_{fw} of 0.172 µg/L and an NC_{sw} of 0.020 µg/L.

3.6 Derivation of the SRC

The base set is complete and NOEC values are available for algae and crustacea. The geometric mean of the combined L(E)C50 values is 8.72 mg/L, the geometric mean value of the NOECs is 1.20 mg/L. The geometric mean of the acute values divided by 10 is smaller than the geometric mean of the NOEC values. Therefore, the $SRC_{water, eco}$ is based on the geometric mean of the LC50 values using an assessment factor of 10. The $SRC_{water, eco}$ is 0.872 mg/L = 872 µg/L. This value is valid for freshwater and saltwater.

4 Derivation of risk limits for soil, groundwater and air

4.1 Derivation of ERLS for soil

4.1.1 Derivation of the MPC

4.1.1.1 Derivation of the $MPC_{soil,\ eco}$

Because no experimental terrestrial ecotoxicity data for xylene are available, the equilibrium partitioning method is used ([6], section 3.7). Using the AA-EQS of 17.2 µg/L, a log Koc of 2.35 and a Henry's law constant of 651 Pa.m^3/mol (geometric mean of values for individual isomers), this results in a $MPC_{soil,\ eco}$ of 229 µg/kg, expressed on the basis of dry soil with Dutch standard conditions (10% organic matter).

4.1.1.2 Derivation of the $MPC_{soil,\ hh}$

Using the TDI of 150 µg/kg bw per day, a Koc of 224 L/kg, Henry coefficient of 651 Pa.m^3/mol, log Kow of 3.14 and water solubility of 194 mg/L (geometric mean of values for individual isomers), the $MPC_{soil,\ hh}$ is calculated as 1811 mg/kg dwt according to the methods in section 3.3.6 of the INS Guidance [6].

4.1.1.3 Selection of the MPC_{soil}

The MPC_{soil} is set to the lowest value of the routes included, and is 229 µg/kg dwt soil at 10% organic matter.

4.1.2 Derivation of the NC

The NC_{soil} is derived by dividing the MPC_{soil} by a factor of 100, resulting in an NC_{soil} of 2.3 µg/kg dwt soil.

4.1.3 Derivation of the SRC

The $SRC_{soil,\ eco}$ is derived similar to the $MPC_{soil,\ eco}$ using equilibrium partitioning. With the $SRC_{water,\ eco}$ of 0.872 mg/L, the $SRC_{soil,\ eco}$ is 11.6 mg/kg dwt for Dutch standard soil with 10% organic matter (11600 µg/kg dwt soil).

4.2 Derivation of ERLs for groundwater

4.2.1 Derivation of the MPC

4.2.1.1 Derivation of the $MPC_{grw,\ eco}$

Since groundwater-specific ecotoxicological data are not available for xylene, the AA-EQS for freshwater is used as a substitute [6]. The $MPC_{grw,\ eco}$ is 17.2 µg/L.

4.2.1.2 Derivation of the $MPC_{grw,\ hh}$

The human health based MPC for groundwater is set equal to the $QS_{dw,\ hh}$. The $MPC_{grw,\ hh}$ is 500 µg/L.

4.2.1.3 Selection of the MPC_{grw}

The MPC_{grw} is set to the lowest value of the routes included, and is 17.2 µg/L.

4.2.2 Derivation of the NC

The NC_{grw} is derived by dividing the MPC_{grw} by a factor of 100, resulting in an NC_{grw} of 0.172 µg/L. This is about equal to the current target value for groundwater of 0.2 µg/L [19].

4.2.3 Derivation of the SRC

Since groundwater-specific ecotoxicological data are not available for xylene, the SRC for freshwater is used as a substitute. The $SRC_{grw, eco}$ is 872 µg/L.

4.3 Derivation of ERLs for air

4.3.1 Derivation of the MPC

The MPC_{air} is derived taking into account the human toxicological risk limits for inhalation (Tolerable Concentration in Air). Ecotoxicological effects due to exposure via air is considered if data indicate that this is a relevant route, but this is not the case. A TCA of 870 µg/m^3 was derived in 2001 [15]. The MPC_{air} is set to 870 µg/m^3.

4.3.2 Derivation of the NC

The NC_{air} is derived by dividing the MPC_{air} by a factor of 100, resulting in an NC_{air} of 8.70 µg/m^3.

5 Conclusions

Updated risk limits for xylenes are derived for fresh and marine surface water, groundwater, soil and air. The update was performed because additional ecotoxicity information on water organisms was available which together with changes in methodology lead to substantially different values. Moreover, it was decided to present ERLs only for the xylenes as a group, because this is most relevant from an ecotoxicological point of view.

The proposed AA-EQS, MAC-EQS and $QS_{dw, hh}$ for surface water and the additional national specific risk limits Negligible Concentration (NC), Maximum Permissible Concentration (MPC), and Serious Risk Concentration for ecosystems (SRC) are summarised in the table below.

Monitoring data reported for o-xylene in surface water indicate that concentrations of this isomer are far below the proposed water quality standards [20]. It should be noted that the sum limits (Table 12) only apply when all three isomers are monitored. Therefore, a definitive conclusion as to whether the new standards will be met can only be drawn on the basis of the summed concentration of the three individual isomers.

Table 12 Derived AA-EQS, MAC-EQS, $QS_{dw, hh}$, MPC, NC, and SRC values for xylene. Values for water are given in two significant digits where appropriate.

Compartment	**Environmental Risk Limit**			
	AA-EQS	**MAC-EQS**	**NC**	**SRC**
Freshwater [μg/L]	17	244	0.17	872
Marine water [μg/L]	1.7	49	0.020	872
Surface water [μg/L] (drinking water abstraction)	500			
	MPC		**NC**	**SRC**
Soil [μg/kg dwt]	229	-	2.3	11600
Groundwater [μg/L]	17	-	0.17	872
Air [μg/m^3]	870	-	8.7	-

- = not applicable

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List of terms and abbreviations

AA-EQS	Annual Average Environmental Quality Standard
BCF	Bioconcentration Factor
BMF	Biomagnification Factor
CLP	Classification Labelling and Packaging of substances
CMR	Carcinogenic, Mutagenic, Reprotoxic
ECHA	European Chemicals Agency
EC_x	Concentration at which x% effect is observed
EQS	Environmental Quality Standard
ER	Ernstig Risiconiveau (= SRC)
ERL	Environmental risk limit
$f_{oc, susp}$	fraction organic carbon in suspended matter
HC5, HC50	Hazardous Concentration for 5%, 50% of the species
INS	International and National Environmental Quality Standards for Substances in the Netherlands
JG-MKN	Jaargemiddelde milieukwaliteitsnorm (= AA-EQS)
Koc	Organic carbon-water partitioning coefficient
Kow	Octanol-water partitioning coefficient
LCx	Concentration at which x% mortality is observed
MAC-EQS	Maximum Acceptable Concentration for ecosystems
$MAC\text{-}EQS_{fw}$	Maximum Acceptable Concentration for ecosystems in freshwater
$MAC\text{-}EQS_{sw}$	Maximum Acceptable Concentration for ecosystems in the saltwater compartment
MAC-MKN	Maximum Aanvaardbare Concentratie milieukwaliteitsnorm (= MAC-EQS)
Marine species	Species that are representative for marine and brackish water environments and that are tested in water with salinity > 0.5 ‰.
MKN	milieukwaliteitsnorm (= EQS)
MPC	Maximum Permissible Concentration
MPC_{air}	Maximum permissible Concentration in air
$MPC_{grw, eco}$	Maximum Permissible Concentration in groundwater, based on ecotoxicity
$MPC_{grw, hh}$	Maximum Permissible Concentration in groundwater, based on human health
$MPC_{soil, eco}$	Maximum Permissible Concentration in soil, based on ecotoxicity
$MPC_{soil, hh}$	Maximum Permissible Concentration in soil, based on human health
MTR	Maximaal Toelaatbaar Risiconiveau (= MPC)
NC	Negligible Concentration
NC_{air}	Negligible Concentration in air
NC_{fw}	Negligible Concentration in freshwater
NC_{grw}	Negligible Concentration in groundwater
NC_{soil}	Negligible Concentration in soil
NC_{sw}	Negligible Concentration in saltwater
NOEC	No Observed Effect Concentration
$QS_{dw, hh}$	Quality standard for water used for abstraction of drinking water
$QS_{fw, eco}$	Quality standard for freshwater based on ecotoxicological data
$QS_{sw, eco}$	Quality standard for saltwater based on ecotoxicological data
REACH	Regulation Registration, Evaluation, Authorisation of Chemicals EC/1907/2006
RIVM	Rijksinstituut voor Volksgezondheid en Milieu (= National Institute for Public Health and the Environment)

SRC	Serious Risk Concentration for ecosystems
SRC_{eco}	Serious Risk Concentration for ecosystems
$SRC_{fw, eco}$	Serious risk concentration for freshwater ecosystems
$SRC_{grw, eco}$	Serious Risk Concentration for ecosystems in groundwater
$SRC_{soil, eco}$	Serious Risk Concentration for ecosystems in soil
$SRC_{sw, eco}$	Serious risk concentration for saltwater ecosystems
$SRC_{water, eco}$	Serious Risk Concentration for ecosystems in water
SSD	Species Sensitivity Distribution
TDI	Tolerable Daily Intake
TGD	Technical Guidance Document
VR	Verwaarloosbaar Risiconiveau (= NC)
WFD	Water Framework Directive (2000/60/EC)
WHO	World Health Organization

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 [mg $CaCO_3$/L]	Temp [°C]	Exposure time	Exp. conc. [mg/L]	BCF [L/kg_{ww}]	Ri	Notes	Reference
Algae														
Pseudokirchneriella subcapitata			GC			23			12h	8.33	251.19	3	1,2	[21]
Scenedesmus quadricauda		GC standard	GC-FID	S	am	7.5		22	96h		37.65	2	3	[22]
Crustacea														
Daphnia spinulata	< 24h	GC standard	GC-FID	S	am	7.8	95.8	20	48h		63.96	2	3	[22]
Hyalella curvispina	10 day	GC standard	GC-FID		dw	8.3	126	21	96h		62.90	2	3	[22]
Mollusca														
Tapes semidecussata			GC-FID	CF			30‰	14	8d	3.1	6.43	2	4	[13]
Pisces														
Anguilla japonica	130-180g		GC-FID					20	10d	50	23.6	2	3	[23]
Carassius auratus			GC-FID	S?						1	14.79	4	5	[14]

Notes
1 Recalculated from µg/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 test type or exposure time, logBCF=1.17

Table A1.2 Bioconcentration of o-xylene

Species	Species properties	Substance purity [%]	Analysed	Test type	Test water	pH	Hardness/ salinity [mg $CaCO_3$/L]	Temp [°C]	Exposure time	Exp. conc. [mg/L]	BCF [L/kg_{ww}]	Ri	Notes	Reference
Algae														
Pseudokirchneriella subcapitata			GC			23			12h	8.33	218.78	3	1, 2	[21]
Scenedesmus quadricauda		GC standard	GC-FID	S	am	7.5		22	96h		9.76	2	3	[22]
Crustacea														
Daphnia spinulata	< 24h	GC standard	GC-FID	S	am	7.8	95.8	20	48h		43.44	2	3	[22]
Hyalella curvispina	10 day	GC standard	GC-FID		dw	8.3	126	21	96h		42.60	2	3	[22]
Mollusca														
Tapes semidecussata			GC-FID	CF			30‰	14	8d	3.1	7.25	2	4	[13]
Pisces														
Anguilla japonica	130-180g		GC-FID					20	10d	50	21.4	2	3	[23]
Carassius auratus			GC-FID	S?						1	14.13	4	5	[14]

Notes
1 Recalculated from µg/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 test type or exposure time, logBCF=1.17

Table A1.3 Bioconcentration of p-xylene

Species	Species properties	Substance purity [%]	Analysed	Test type	Test water	pH	Hardness/ salinity [mg $CaCO_3$/L]	Temp [°C]	Exposure time	Exp. conc. [mg/L]	BCF [L/kg_{ww}]	Ri	Notes	Reference
Algae														
Pseudokirchneriella subcapitata			GC			23			12h	8,33	257.04	3	1,2	[21]
Scenedesmus quadricauda		GC standard	GC-FID	S	am	7.5		22	96h		26.60	2	3	[22]
Crustacea														
Daphnia spinulata	< 24h	GC standard	GC-FID	S	am	7.8	95.8	20	48h		60.60	2	3	[22]
Hyalella curvispina	10 day	GC standard	GC-FID		dw	8.3	126	21	96h		58.34	2	3	[22]
Pisces														
Anguilla japonica	130-180g		GC-FID					20	10d	50	23.6	2	3	[23]
Carassius auratus			GC-FID	S?						1	14.79	4	4	[14]

Notes
1 Recalculated from µg/kg
2 BTEX mixture used for exposure
3 Exposure in crude oil suspension
4 No data on test type or exposure time, logBCF=1.17

Appendix 2. Detailed toxicity data

Legend to column headings	
A	test water analysed y(es)/n(o)
Test type	S = static; R = renewal; F = flow through; c = closed
Purity	refers to purity of active substance or content of active substance in formulation; GC standard= gaschromatogrphy; ag = analytical grade; tg = technical grade
Test water	am = artificial medium; dtw = dechlorinated tap water; dw = deionised/dechlorinated/distilled water; nw = natural water; rw = reconstituted water; rtw = reconstituted tap water; tw = tap water
T	temperature
Ri	Reliability index according to [9]. Valid studies (Ri 2 or higher) are considered for EQS-derivation, depending on relevance and considering notes on data treatment

Table A.2.1 Acute toxicity of m-xylene to freshwater organisms

Species	Species properties	A	Test type	Purity [%]	Test water	pH	T [°C]	Hardness as $CaCO_3$ [mg /L]	Exp. time	Criterion	Test endpoint	Value [mg/L]	Ri	Notes	Reference
Protozoa															
Tetrahymena pyriformis	stat. phase		S		am		28	20	24h	LC100	Mortality	399.60	3	3,17	[24] in [12]
Algae															
Scenedesmus quadricauda		y	S	GC std.	am	7.5	22		96h	EC50	Growth	7.43	2	4,6,8	[22]
Pseudokirchneriella subcapitata	log phase		S		am	7			8d	EC50	Growth	3.90	3	7	[25] in [12]
Pseudokirchneriella subcapitata		n	Sc?	GC std.					72h	EC50	Growth	4.90	3	2,4,8	[26]
Crustacea															
Cerodaphnia cf. dubia		y	Sc	>97		7.7		65.2	48h	EC50	Immobilisation	2.44	2	9,10,11	[27]
Daphnia magna	24h	y	Sc		am	7.2-8	20	250	48h	LC50	Mortality	36.26	2	19	[28]
Daphnia magna	juvenile (4-6 day)		S			6-7	23		48h	LC50	Mortality	9.56	4*		[29] in [12]
Daphnia magna	4 - 6 days	n	Sc	>97	dw	6.5	23		48h	LC50	Mortality	9.55	3	12	[29]
Daphnia magna		y	Sc	GC std.					24h	IC50	Immobilisation	4.70	2	2,4,8	[26]
Daphnia magna	6-24h old		Sc	>95	dw		22		24h	IC50	Immobilisation	23.77	2	13	[30]
Daphnia spinulata	< 24h	y	S	GC std.	am	7.8	20	95.8	48h	LC50	Mortality	4.25	2	4,8,14,15	[22]
Hyalella curvispina	10 day	y	S	GC std.	dw	8.3	21	82	96h	LC50	Mortality	4.25	2	4,8,15	[22]
Pisces															
Bryconamericus iberingii	4.7 cm. 2.85g	y	Sc	GC std.	nw	7.9	20	98	96h	LC50	Mortality	11.68	1	2,4,8,16	[22]
Bryconamericus iberingii	2.85g. 4.7cm	y	Sc	GC std.					96h	LC50	Mortality	11.23	2	2,4,8	[31]
Carassius auratus									96h	LC50	Mortality	16.00	4		[12]
Carassius auratus	6.2 cm.	y	S		tw	6-7	20		24h	LC50	Mortality	16.00	2	1,4	[32]
Cnesterodon decemmaculatus		y	Sc	GC std.	dw	8.59	19.5	141.6	96h	LC50	Mortality	10.72	2	2,4,5,8,18	[33]
Oncorhynchus mykiss		y	R	GC std.			12		96h	LC50	Mortality	8.40	2	2,5,8	[26]
Oryzias latipes			R		tw	7.2	20 ± 1		96 h	LC50	Mortality	32.00	2	2	[34]
Pimephales promelas		y	Sc	GC std.				46	96h	LC50	Mortality	15.49	2	2,4,8	[33]
Poecilia reticulata		y	R	GC std.			21		96h	LC50	Mortality	12.90	2	2,5,8	[26]
Poecilia reticulata	2-3 m	n	R		tw		22	25	14d	LC50	Mortality	37.67	3	1	[35]

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 µmol/L
12 Recalculated from mmol/m^3
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]	Ri	Notes	Reference
Bacteria															
Vibrio fischeri			Sc	>95	dw		20	3% NaCl	15m	EC50	Luminescence	19.31	2	1	[30]
Crustacea															
Artemia salina		y	Sc		aw	8-8.3	21.5-23	30	48h	LC50	Mortality	10.80	2	5	[28]
Artemia salina		y	Sc		aw	8-8.3	21.5-23	30	48h	EC50	Immobilisation	7.85	2	6	[28]
Artemia salina		n	Sc	>97			20	30	24h	LC50	Mortality	19.32	3	2	[36]
Crago franciscorum	1.8g	y	S	>99	nw		16	25	96h	LC50	Mortality	3.70	3	3	[37]
Pisces															
Gadus morrhua	eggs		S	>98,5	sea		4-6	34	6h	40-50% increase of mortality	Mortality	16-35	3	4	[38] in [12]
Morone saxatilis	6.0g	y	S	>99	nw		16	25	96h	LC50	Mortality	9.20	3	3	[37]

Notes
1 Recalculated from log1/value (3.74 mol/L)
2 Methods in Wells et al 1982, value recalculated from mmoL/m^3
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
6 Geomean of 8.54, 10.9, 7.09, 5.75

Table A.2.3 Chronic toxicity of m-xylene to freshwater organisms

Species	Species properties	A	Test type	Purity [%]	Test water	pH	T [°C]	Hardness as $CaCO_3$ [mg /L]	Exp. time	Criterion	Test endpoint	Value [mg/L]	Ri	Notes	Reference
Algae															
Pseudokirchneriella subcapitata		y	Sc			neutral			8d	NOEC	Growth	0.7	2	1	[25]
Crustacea															
Ceriodaphnia dubia		y	Rc	>99		7.6		68.3	7d	NOEC	Reproduction	1.2	2	2	[39]

Notes
1 16h/8h light/dark cycle; value based on measured concentrations; unclear when analysis is performed
2 Test according to US EPA Whole Effluent Testing Program; 16h/8h light/dark cycle; daily renewal, actual concentrations 86% of nominal; individual data provided; endpoint based on nominal concentration, recalculated from reported value of 11 µM.

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

Species	Species properties	A	Test type	Purity [%]	Test water	pH	T [°C]	Hardness as $CaCO_3$ [mg /L]	Exp. time	Criterion	Test endpoint	Value [mg/L]	Ri	Notes	Reference
Algae															
Pseudokirchneriella subcapitata		y	Sc?	GC std.					72h	EC50	Growth	4.70	2	1,2,4	[26]
Scenedesmus quadricauda		y	S	GC std.	am	7.5	22		96h	EC50	Growth	27.60	2	2,4,8	[22]
Crustacea															
Daphnia magna	24h	y	Sc		am	7.8-8.1	19.5-22	250	48h	LC50	Mortality	17.43	2	17	[28]
Daphnia magna	4 - 6 days	n	Sc	97	dw	6.5	23		48h	LC50	Mortality	3.18	3	5	[29]
Daphnia magna		y	Sc	GC std.					24h	IC50	Immobilisation	1.00	2	1,2,4	[26]
Daphnia magna	<24h	y	CF		nw	7.39	17	44.7	48h	LC50	Mortality	3.82	2		[40]
Daphnia magna					dw					LC50	Mortality	>100. <1000	4		[41]
Daphnia magna	6-24h old		Sc	>95	dw		22		24h	IC50	Immobilisation	17.22	2	9	[30]
Daphnia spinulata	< 24h	y	S	GC std.	am	7.8	20	95.8	48h	LC50	Mortality	6.37	2	2,4,6,10	[22]
Hyalella curvispina	10 day	y	S	GC std.	dw	8.3	21	82	96h	LC50	Mortality	6.37	2	2,4,10	[22]
Amphibiae															
Xenopus laevis	larvae		Sc		TW		20		48h	LC50	Mortality	73.00	4		[12]
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	[22]
Bryconamericus iheringii	4.7 cm. 2.85g	y	Sc	GC std.					96h	LC50	Mortality	9.94	2	1,2,4	[31]
Carassius auratus	6.2 cm. 3.3 g	y	S		tw	6-7	20		24h	LC50	Mortality	13.00	3	2,2	[32]
Carassius auratus	2.5g	y	CF		nw	7.39	17	44.7	48h	LC50	Mortality	16.10	2	12	[40]
Catostomus commersoni	2.4g	y	CF		nw	7.39	17	44.7	48h	LC50	Mortality	16.10	2	12	[40]
Cnesterodon decemmaculatus		y	Sc	GC std.	dw	8.59	19.5	141.6	96h	LC50	Mortality	9.33	2	1,2,3,4,16	[33]
Lepomis macrochirus	1.1	y	CF		nw	7.39	17	44.7	48h	LC50	Mortality	16.10	2	12	[40]
Oncorhynchus mykiss		y	R	GC std.			12		96h	LC50	Mortality	7.60	2	1,3,4	[26]
Oncorhynchus mykiss	13.1g	y	CF		nw	7.39	17	44.7	48h	LC50	Mortality	8.05	2	12	[40]
Pimephales promelas	0.3	y	CF		nw	7.39	17	44.7	48h	LC50	Mortality	16.10	2	13	[40]
Pimephales promelas		y	Sc	GC std.					96h	LC50	Mortality	16.22	2	1,2	[33]
Pimephales promelas	4-6wks. 1.1-3.1 cm	n	S		dw		18-22		96h	LC50	Mortality	42.00	3	14	[42]
Poecilia reticulata		n	S				22	25	7d	LC50	Mortality	35.00	3*		[12]
Poecilia reticulata		y	R	GC std.			21		96h	LC50	Mortality	12.00	2	1,3,4	[26]
Poecilia reticulata	2-3 months	n	R		tw		22	25	7d	LC50	Mortality	35.15	3	15	[35]

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/m^3
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]	Ri	Notes	Reference
Bacteria															
Vibrio fischeri										EC50	Bioluminescence	9.25	2	1	[43]
Vibrio fischeri		n	S		am		15	20	15m	EC20	Bioluminescence	16.67	3	7	[44]
Vibrio fischeri			Sc	>95	dw		20	3% NaCl	15m	EC50	Luminescence	8.83	2	5	[30]
Crustacea															
Artemia		y	Sc		aw	8.3-8.4	19.5-22	30	48h	LC50	Mortality	24.64	2	6	[28]
Artemia		y	Sc		aw	8.3-8.4	19.5-22	30	48h	EC50	Immobilization	11.7	2	8	[28]
Artemia		n	Sc	>97			20	30	24h	LC50	Mortality	23.67	3	2	[36]
Crago franciscorum	1.8g	y	S	>99	nw		16	25	96h	LC50	Mortality	1.30	3	3	[37]
Cancer magister dana	larvae	n	S				13	30	48h	LC50	Mortality	38.00	4		[12]
Echinodermata															
Strongylocentrotus droebachiensis	eggs; first day after fertilisation	y	S	>98	nw				96h	EC50		4.10	2	4	[45]
Pisces															
Morone saxatilis	6.0g	y	S	>99	nw		16	25	96h	LC50	Mortality	11.00	3	3	[37]

Notes
1 Microtox test
2 Methods in Wells et al 1982, value recalculated from mmol/m^3
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
8 Geomean of 12.7 and 10.7

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

Species	Species properties	A	Test type	Purity [%]	Test water	pH	T [°C]	Hardness as $CaCO_3$ [mg /L]	Exp. time	Criterion	Test endpoint	Value [mg/L]	Ri	Notes	Reference
Algae															
Pseudokirchneriella subcapitata		y	Sc			neutral			8d	NOEC	Growth	1	2	1	[25]
Chlorella vulgaris	30000 cells/mL	n	Sc		am		20		24h	EC10	Growth rate	12.47	3	2	[46]

Notes
1 16h/8h light/dark cycle; value based on measured concentrations; unclear when analysis is performed
2 test duration too short

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

Species	Species properties	A	Test type	Purity [%]	Test water	pH	T [°C]	Hardness as $CaCO_3$ [mg /L]	Exp. time	Criterion	Test endpoint	Value [mg/L]	Ri	Notes	Reference
Protozoa															
Tetrahymena pyriformis		n	S	>95	am	7.35	27		48h	IC50	Growth	88.10	3	1	[24]
Algae															
Chlamydomonas sp.									3h	EC50	Inhib. photosyn.	45.70	4		[12]
Chlorella vulgaris		n							3h	EC50	Inhib. photosyn.	105.10	4		[12]
Pseudokirchneriella subcapitata		y	Sc?	GC std					72h	EC50	Growth	3.20	2	2,3,5	[26]
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	[22]
Crustacea															
Daphnia magna	24h	y	Sc		am	7.4-7.9	20.5-21	250	48h	LC50	Mortality	32.24	2	15	[28]
Daphnia magna	4 - 6 days	n	Sc	>97	dw	6.5	23		48h	LC50	Mortality	8.49	2	6	[29]
Daphnia magna			Sc	GC std					24	IC50	Immobilisation	3.60	2	2,3,5	[26]
Daphnia magna	6-24h old		Sc	>95	dw		22		24h	IC50	Immobilisation	22.18	2	11	[30]
Daphnia spinulata	< 24h	y	S	GC std	am	7.8	20	95.8	48h	LC50	Mortality	4.25	2	3,7,8	[22]
Hyalella curvispina	10 day	y	S	GC std	dw	8.3	21	82	96h	LC50	Mortality	4.25	2	3,8	[22]
Rotifera															
Brachionus calyciflorus			S		rw	7.5	25		24h	LC50	Mortality	253.00	3	13	[47]
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	[22]
Bryconamericus iheringii	2.85g. 4.7cm	y	Sc	GC std					96h	LC50	Mortality	6.90	2	2,3,5	[31]
Carassius auratus	6.2 cm. 3.3 g	y	S		tw	6-7	20		24h	LC50	Mortality	18.00	3	1,3	[32]
Cnesterodon decemmaculatus		y	Sc	GC std	dw	8.59	19.5	141.6	96h	LC50	Mortality	6.17	2	2,3,4,14	[31]
Oncorhynchus mykiss		y	R	GC std			12		96h	LC50	Mortality	2.60	2	2,4,5	[26]
Pimephales promelas		y	Sc	GC std					96h	LC50	Mortality	8.91	2	2,3,5	[33]
Pimephales promelas	44 g, 35 mm	y	Fc	99.7		7	22-24	37-40	96 h	LC50	mortality	4.7	2	2,5,16	REACH dossier
Poecilia reticulata		y	R	GC std			21		96h	LC50	Mortality	8.80	2	2,4,5	[26]
Poecilia reticulata	2-3 mo	n	R		tw		22	25	7d	LC50	Mortality	35.15	3	12	[35]

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
16 Data from public REACH summary dossier p-xylene; summary includes detailed information on test conditions and results, therefore accepted

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]	Ri	Notes	Reference
Bacteria															
Vibrio fischeri			Sc	>95	dw		20	3% NaCl	15m	EC50	Luminescence	17.22	2	3	[30]
Crustacea															
Artemia		y	Sc		aw	8.1-8.2	21-22.5	30	24h	LC50	Mortality	27.80	2		[28]
Artemia		y	Sc		aw	8.1-8.2	21-22.5	30	24h	EC50	Immobilisation	18.4	2	4	[28]
Artemia		n	Sc	>97			20	30	24h	LC50	Mortality	24.63	3	1	[36]
Crago franciscorum	1.8g	y	S	>99	nw		16	25	96h	LC50	Mortality	2.00	3	2	[37]
Pisces															
Morone saxatilis	6.0g	y	S	>99	nw		16	25	96h	LC50	Mortality	2.00	3	2	[37]

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)
4 geometric mean of 20.6 and 16.5

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

Species	Species properties	A	Test type	Purity [%]	Test water	pH	T [°C]	Hardness as $CaCO_3$ [mg /L]	Exp. time	Criterion	Test endpoint	Value [mg/L]	Ri	Notes	Reference
Algae															
Pseudokirchneriella subcapitata		y	Sc			neutral			8d	NOEC	Growth	0.9	2	1	[25]
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	2	[48]
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	2	[48]
Crustacea															
Daphnia magna	<24 h	y	R	99.4	am	7.5-8.7	20		21 d	NOEC	Reproduction	1.57	1	2	[49]
Daphnia magna	<24 h	y	R	99.4	am	7.5-8.7	20		21 d	EC10	Reproduction	1.91	1	2	[49]

Notes
1 16h/8h light/dark cycle; value based on measured concentrations; unclear when analysis is performed
2 OECD, GLP; based on measured concentrations

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