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Rapport in het kort

Milieurisicogrenzen voor 1,3-butadieen

Dit rapport geeft milieurisicogrenzen voor 1,3-butadieen in (grond)water, bodem en lucht. Milieurisicogrenzen zijn de technisch-wetenschappelijke advieswaarden voor de uiteindelijke milieukwaliteitsnormen in Nederland. De milieurisicogrenzen voor 1,3-butadieen zijn gebaseerd op de uitkomsten van de EU risicobeoordeling voor 1,3-butadieen (Bestaande Stoffen Verordening 793/93). De afleiding van de milieurisicogrenzen sluit tevens aan bij de richtlijnen uit de Kaderrichtlijn Water. Monitoringsgegevens voor Nederland zijn niet beschikbaar, daarom kan er geen verwachting worden uitgesproken of de afgeleide milieurisicogrenzen in Nederland overschreden zullen worden.

Trefwoorden: milieukwaliteitsnormen; milieurisicogrenzen; 1,3-butadieen; maximaal toelaatbaar risiconiveau; verwaarloosbaar risiconiveau

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Contents

Summary

Environmental risk limits (ERLs) are derived using ecotoxicological, physico-chemical, and human toxicological data. They represent environmental concentrations of a substance offering different levels of protection to man and ecosystems. It should be noted that the ERLs are scientifically derived values. They serve as advisory values for the Dutch Steering Committee for Substances, which is appointed to set the Environmental Quality Standards (EQSs) from these ERLs. ERLs should thus be considered as preliminary values that do not have any official status.

This report contains ERLs for 1,3-butadiene in water, groundwater, soil and air. The following ERLs are derived: negligible concentration (NC), maximum permissible concentration (MPC), maximum acceptable concentration for ecosystems (MAC_{eco}), and serious risk concentration for ecosystems (SRC_{eco}). The risk limits were solely based on data presented in the Risk Assessment Reports (RAR) for this compound, prepared under the European Existing Substances Regulation (793/93/EEC). No risk limits were derived for the sediment compartment, because of the relatively low sediment-water partition coefficient. Because of the physical nature of the substance, its high vapour pressure and flammable nature, it would be very difficult to test meaningfully and no experimental aquatic toxicity data are available. Therefore, QSAR derived aquatic toxicity data have been used in the derivation of the ERLs. Because of this reason, there is a higher uncertainty in the derived values than when experimental aquatic toxicity data are used.

For the derivation of the MPC and MAC_{eco} for water, the methodology used is in accordance with the Water Framework Directive. This methodology is based on the Technical Guidance Document on risk assessment for new and existing substances and biocides (European Commission (Joint Research Centre), 2003). For the NC and the SRC_{eco}, the guidance developed for the project 'International and National Environmental Quality Standards for Substances in the Netherlands' was used (Van Vlaardingen and Verbruggen, 2007). An overview of the derived environmental risk limits is given in Table 1.

Monitoring data for 1,3-butadiene in the Dutch environment are not available. Therefore it cannot be judged if the derived ERLs are being exceeded.

Table 1. Derived MPC, NC, MAC_{eco}, and SRC_{eco} values for 1,3-butadiene.

ERL	**unit**	**value**			
		MPC	NC	MAC_{eco}	SRC_{eco}
water [a]	$ng.L^{-1}$	62	0.62	3.3×10^{5} [d]	3.7×10^{6} [d]
drinking water [b]	$ng.L^{-1}$	35			
marine	$ng.L^{-1}$	62	0.62	3.3×10^{4} [d]	3.7×10^{6} [d]
sediment	$mg.kg_{dwt}^{-1}$	n.d.			
soil [c]	$\mu g.kg_{dwt}^{-1}$	0.36	3.6×10^{-3}		1.7×10^{4} [e]
groundwater	$ng.L^{-1}$	35	0.35		3.7×10^{6} [d]
air	$ng.m^{-3}$	30	0.30		

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

[b] The exact way of implementation of the $MPC_{dw, water}$ in the Netherlands is at present under discussion. Therefore, the $MPC_{dw, water}$ is presented as a separate value in this report.

[c] Expressed on the basis of Dutch standard soil.

[d] Value based on QSARs for toxicity.

[e] Value based on QSARs for toxicity and equilibrium partitioning.

n.d. = not derived.

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1 Introduction

1.1 Project framework

In this report environmental risk limits (ERLs) for surface water (freshwater and marine), soil and groundwater are derived for 1,3-butadiene. The following ERLs are considered:

- Negligible Concentration (NC) – concentration at which effects to ecosystems are expected to be negligible and functional properties of ecosystems must be safeguarded fully. It defines a safety margin which should exclude combination toxicity. The NC is derived by dividing the MPC (see next bullet) by a factor of 100.
- Maximum Permissible Concentration (MPC) – concentration in an environmental compartment at which:
  1. no effect to be rated as negative is to be expected for ecosystems;
  2a no effect to be rated as negative is to be expected for humans (for non-carcinogenic substances);
  2b for humans no more than a probability of 10^{-6} over the whole life (one additional cancer incident in 10^6 persons taking up the substance concerned for 70 years) can be calculated (for carcinogenic substances) (Lepper, 2005).
- Maximum Acceptable Concentration (MAC_{eco}) – concentration protecting aquatic ecosystems for effects due to short-term exposure or concentration peaks.
- Serious Risk Concentration (SRC_{eco}) – concentration at which serious negative effects in an ecosystem may occur.

It should be noted that ERLs are scientifically derived values based on (eco)toxicological, fate and physico-chemical data. They serve as advisory values for the Dutch Steering Committee for Substances, which is appointed to set the Environmental Quality Standards (EQSs) from these ERLs. ERLs should thus be considered as preliminary values that do not have any official status.

1.2 Production and use of 1,3-butadiene

The Risk Assessment Report (RAR) (European Commission, 2002) reports that the most widely used production method for 1,3-butadiene is recovery from a by-product stream during the production of ethylene. The total production capacity reported is between 1.2 and 5.0 million tonnes per year. 1,3-Butadiene is used in closed systems as an intermediate for polymerisation and copolymerisation. The major use is for the production of synthetic rubber, thermoplastic resins and latex. More information can be found in the RAR (European Commission, 2002).

2 Methods

2.1 Data collection

The final Risk Assessment Report (RAR) of 1,3-butadiene (European Commission, 2002) produced in the framework of Existing Substances Regulation (793/93/EEC) was used as only source of physico-chemical and (eco)toxicity data. Information given in the RARs is checked thoroughly by European Union member states (Technical Committee) and afterwards approved by the Scientific Commission on Health and Environmental Risk (SCHER). Therefore, no additional evaluation of data is performed for the ERL derivation. Only valid data combined in an aggregated data table are presented in the current report. Occasionally, key studies are discussed when relevant for the derivation of a certain ERL.

In the aggregated data table only one effect value per species is presented. When for a species several effect data are available, the geometric mean of multiple values for the same endpoint is calculated where possible. Subsequently, when several endpoints are available for one species, the lowest of these endpoints (per species) is reported in the aggregated data table.

2.2 Methodology for derivation of environmental risk limits

The methodology for data selection and ERL derivation is described in Van Vlaardingen and Verbruggen (2007) which is in accordance with Lepper (2005). For the derivation of ERLs for air, no specific guidance is available. However, as much as possible the basic principles underpinning the ERL derivation for the other compartments are followed for the atmospheric ERL derivation (if relevant for a chemical).

2.2.1 Drinking water abstraction

The INS-Guidance includes the MPC for surface waters intended for the abstraction of drinking water ($MPC_{dw, water}$) as one of the MPCs from which the lowest value should be selected as the general MPC_{water} (see INS-Guidance, Section 3.1.6 and 3.1.7). According to the proposal for the daughter directive Priority Substances, however, the derivation of the AA-EQS (= MPC) should be based on direct exposure, secondary poisoning, and human exposure due to the consumption of fish. Drinking water was not included in the proposal and is thus not guiding for the general MPC_{water} value. The exact way of implementation of the $MPC_{dw, water}$ in the Netherlands is at present under discussion within the framework of the "AMvB Kwaliteitseisen en Monitoring Water". No policy decision has been taken yet, and the $MPC_{dw, water}$ is therefore presented as a separate value in this report.

The $MPC_{dw, water}$ is also used to derive the MPC_{gw}. For the derivation of the $MPC_{dw, water}$, a substance specific removal efficiency related to simple water treatment may be needed. Because there is no agreement as yet on how the removal fraction should be calculated, water treatment is not taken into account.

2.2.2 $MAC_{eco, marine}$

In this report, a MAC_{eco} is also derived for the marine environment. The assessment factor for the $MAC_{eco, marine}$ value is based on:

- the assessment factor for the $MAC_{eco, water}$ value, when acute toxicity data for at least two specific marine taxa are available, or
- using an additional assessment factor of 5, when acute toxicity data for only one specific marine taxon are available (analogous to the derivation of the MPC according to Van Vlaardingen and Verbruggen (2007)), or
- using an additional assessment factor of 10, when no acute toxicity data are available for specific marine taxa.

If freshwater and marine data sets are not combined the $MAC_{eco, marine}$ is derived on marine toxicity data using the same additional assessment factors as mentioned above. It has to be noted that this procedure is currently not agreed upon. Therefore, the $MAC_{eco, marine}$ value needs to be re-evaluated once an agreed procedure is available.

3 Derivation of environmental risk limits for 1,3-butadiene

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

3.1.1 Identity

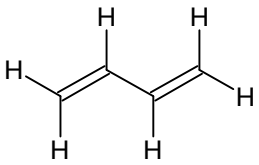


Figure 1. Structural formula of 1,3-butadiene.

Table 2. Identification of 1,3-butadiene.

Parameter	Name or number
Common/trivial/other name	alpha-gamma-butadiene, biethylene, bietileno, bivinile, bivinyl, bivinylerythrene, butadien, butadiene, butadiene-1,3, buta-1,3-diene, diethylene, divinilo, divinyl, eritrene, erythrene, pyrrolylene, trans-butadiene, viniletilene, viniletileno, vinylethylen, vinylethylene
CAS number	106-99-0
EC number	203-450-8
Molecular formula:	C_4H_6
Smiles	C(C=C)=C

3.1.2 Physico-chemical properties

Table 3. Physico-chemical properties of 1,3-butadiene.

Parameter	Unit	Value	Remark
Molecular weight	[g.mol^{-1}]	54.09	
Water solubility	[g.L^{-1}]	0.735	at 20 ºC
log K_{OW}	[-]	1.99	experimental data
K_{OC}	[L.kg^{-1}]	51.6	estimated from K_{ow} according to TGD
Vapour pressure	[Pa]	240 x 10^3	at 20 ºC
Melting point	[°C]	-108.9	
Boiling point	[°C]	-4.4	
Henry's law constant	[Pa.m^3.mol^{-1}]	7.4 x 10^3	at 20 °C, estimation based on solubility

n.a. = not applicable.

3.1.3 Behaviour in the environment

Table 4. Selected environmental properties of 1,3-butadiene.

Parameter	Unit	Value	Remark	Reference
Hydrolysis half-life	DT50 [d]		Not expected	RAR
Photolysis half-life	DT50 [d]		Insignificant compared to photooxidation*	RAR
Degradability			Insufficient data available	RAR

*For photooxidation the atmospheric half-life for 1,3-butadiene is 5.8 hours based on atmospheric radical concentrations of 5 x 10^5 molecule.cm^{-3}.

3.1.4 Bioconcentration and biomagnification

An overview of the bioaccumulation data for 1,3-butadiene is given in Table 5.

Table 5. Overview of bioaccumulation data for 1,3-butadiene.

Parameter	Unit	Value	Remark	Reference
BCF (fish)	[$L.kg^{-1}$]	9.8	Based on QSAR	RAR
BMF	[$kg.kg^{-1}$]	1	default value since the BCF < 2000 $L.kg^{-1}$	

3.1.5 Human toxicological threshold limits and carcinogenicity

Classification and labelling according to the 25th ATP of Directive 67/548/EEC:
Classification: F+, R12, R45, R46
Labelling: F+, T, R45, R46, R12, S53, S45

In the RAR it is concluded that the critical toxic effects of 1,3-butadiene are mutagenicity and carcinogenicity. Based on available evidence the compound should be regarded as a potential genotoxic carcinogen in humans (non-threshold carcinogen), the RAR concludes. In the RAR, however, no quantification of the cancer risk is presented. Health Canada (2000), WHO (2001) and US-EPA (2002) do provide quantitative cancer risk assessements. TC_{01}/LEC_{01}-values (tumorigenic concentration associated with a 1% increase in the incidence of or mortality due to cancer) were calculated both from available animal studies and from epidemiological data. The value derived from human data was considered the most reliable estimate of cancer risk. WHO (2001) and Health Canada (2000) calculated a TC_{01} of 1.7 $mg.m^{-3}$ from an epidemiological study showing a relation between exposure to 1,3-butadiene in the styrene-butadiene rubber industry and the development of leukemia. The US EPA used the same study to derive a unit risk of 3 x 10^{-5} per $\mu g.m^{-3}$, using linear extrapolation from an LEC_{01} and an adjustment factor of 2. The latter was applied because animal studies indicated that male-only studies may underestimate the risk to the general population. The unit risk as derived by US EPA (2002) corresponds to an excess lifetime 1 x 10^{-6} cancer risk level of 0.03 $\mu g/m^3$. This value is adopted as the human inhalation limit value.

No oral toxicity studies of 1,3-butadiene are available for the derivation of an oral limit value. In absence of oral data showing otherwise, it must be assumed that 1,3-butadiene will exert genotoxic and carcinogenic effects via this route as well. Quantifying this oral risk is possible using the inhalation estimate. The inhalation limit value of 0.03 $\mu g/m^3$ can be converted to a daily oral dose of

0.01 µg.kg_{bw}^{-1}.day^{-1} (rounded value, calculated using a daily ventilation volume of 20 m^3 for a 70 kg adult). This value is adopted here as oral limit value.

3.2 Trigger values

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

Table 6. 1,3-Butadiene: collected properties for comparison to MPC triggers.

Parameter	Value	Unit	Method/Source
Log $K_{p,susp\text{-}water}$	0.71	[-]	$K_{OC} \times f_{OC,susp}$ [1]
BCF	9.8	[$L.kg^{-1}$]	
BMF	1	[$kg.kg^{-1}$]	
Log K_{OW}	1.99	[-]	
R-phrases	45, 46, 12	[-]	
A1 value	n.a.	[$\mu g.L^{-1}$]	
DW standard	n.a.	[$\mu g.L^{-1}$]	

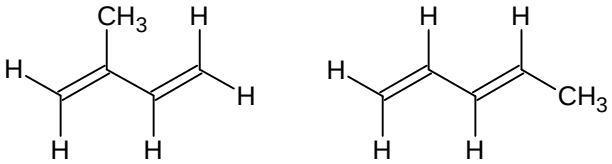
1 $f_{OC,susp}$ = 0.1 $kg_{OC}.kg_{solid}^{-1}$ (European Commission (Joint Research Centre), 2003).

- 1,3-butadiene has a log $K_{p,\ susp\text{-}water} <$ 3; derivation of $MPC_{sediment}$ is not triggered.
- 1,3-butadiene has a log $K_{p,\ susp\text{-}water} <$ 3; expression of the MPC_{water} as $MPC_{susp,\ water}$ is not required.
- 1,3-butadiene has a log $K_{ow} <$ 3; assessment of secondary poisoning is not triggered.
- 1,3-butadiene has an R45 and R46 classification. Therefore, an MPC_{water} for human health via food (fish) consumption ($MPC_{hh\ food,\ water}$) should be derived.

3.3 Toxicity data and derivation of ERLs for water

In the RAR it is reported that no valid aquatic toxicity tests have been carried out using 1,3-butadiene.The lack of experimental aquatic toxicity results for 1,3-butadiene is in line with the physical nature of the substance. Due to its high vapour pressure and flammable nature it would be very difficult to test meaningfully. In the absence of experimental toxicity data, two approaches have been taken in the RAR. Firstly, the toxicity of 1,3-butadiene is estimated using suitable quantitative structure-activity relationships (QSAR); and secondly, toxicity data from structurally similar substances was used to assess the likely toxicity of 1,3-butadiene.

The RAR reports toxicity results for two structurally similar chemicals, isoprene (2-methyl-1,3-butadiene) and 1,3-pentadiene (Figure 2). QSARs from the TGD have been used to calculate chronic and acute data of 1,3-butadiene for algae, *Daphnia* and fish. For comparison the same QSARs have been used to calculate toxicity data for isoprene (2-methyl-1,3-butadiene) and 1,3-pentadiene. The results are given in table 7 and 8.



isoprene 1,3-pentadiene

Figure 2 Structural formula of isoprene and 1,3-pentadiene.

Table 7. QSAR derived freshwater toxicity data for 1,3-butadiene as reported in the RAR.

Chronic		**Acute**	
Taxonomic group	**NOEC (mg.L^{-1})**	**Taxonomic group**	**L(E)C$_{50}$ (mg.L^{-1})**
		Algae	
		algae	32.6
Crustacea		**Crustacea**	
Daphnia magna	6.2	*Daphnia magna*	33.3
Pisces		**Pisces**	
Danio rerio and *Pimephales promelas*	4.4	*Pimephales promelas*	44.8

Table 8. Freshwater toxicity data for chemicals structurally similar to 1,3-butadiene.

Chronic		**Acute**	
Taxonomic group	**NOEC (mg.L^{-1})**	**Taxonomic group**	**L(E)C$_{50}$ (mg.L^{-1})**
1,3-pentadiene		**1,3-pentadiene**	
Algae		**Algae**	
algae	40.9	algae	174.6
		algae QSAR	20.1 and 127*
		Crustacea	
		Daphnia	221.5
		Daphnia QSAR	21.3 and 123*
		Fish	
		fish	139.9
		fish QSAR	30.8 and 147
Isoprene		**Isoprene**	
		Algae	
		Scenedesmus quadricauda	>1000
		algae QSAR	20.1
		Crustacea	
		Daphnia magna	140
		daphnia QSAR	21.3
		Fish	
		Carassius auratus	180
		Lebistes reticulate	240
		Lepomis macrochirus	42.5
		Pimephales promelas	80.4**
		fish QSAR	30.8

*Values calculated with log K_{ow} of 2.3 and 1.5 respectively.
**Geometric mean of 74.8 and 86.5 mg.L^{-1}.

3.3.1 Treatment of fresh- and saltwater toxicity data

Since there are no data for marine species, marine ERLs will be based on freshwater data.

3.3.2 Mesocosm studies

No mesocosm studies are presented in the RAR.

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

3.3.3.1 $MPC_{eco, water}$ and $MPC_{eco, marine}$

In the RAR it is stated that the structurally similar compounds isoprene and 1,3-pentadiene are slightly less toxic than expected from QSAR predictions. Therefore, in the absence of experimental data for 1,3-butadiene it was proposed to base the PNEC on the acute L(E)C50 QSAR predictions with an assessment factor of 1,000 and the long-term NOEC QSAR predictions with an assessment factor of 100. This approach produced a $PNEC_{water}$ of 32.6 $\mu g.L^{-1}$ from the acute QSAR data and 44 $\mu g.L^{-1}$ from the long-term NOEC QSAR data. As a conservative approach, the lower $PNEC_{water}$ of 32.6 $\mu g.L^{-1}$ is used in the assessment. This PNEC is taken over as the $MPC_{eco, water}$, which is therefore: 32.6 $\mu g.L^{-1}$.

The $MPC_{eco, marine}$ using the same data is set a factor 10 lower than the $MPC_{eco, water}$. The $MPC_{eco, marine}$ is: 3.3 $\mu g.L^{-1}$.

3.3.3.2 $MPC_{sp, water}$ and $MPC_{sp, marine}$

1,3-Butadiene has a log $K_{ow} < 3$, thus assessment of secondary poisoning is not triggered.

3.3.3.3 $MPC_{hh\ food, water}$

Derivation of $MPC_{hh\ food, water}$ for 1,3-butadiene is triggered because it is a suspected carcinogen and mutagen (Table 6). The derivation is based on the oral limit value of 0.01 $\mu g.kg_{bw}^{-1}.day^{-1}$. $MPC_{hh, food}$ = 0.1 x 0.01 x 70 / 0.115 = 0.61 $\mu g.kg_{feed}^{-1}$. The resulting $MPC_{hh\ food, water}$ is then: 0.61 / (9.8 x 1) = 0.062 $\mu g.L^{-1}$

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

The MPC_{water} will be the lowest MPC_{water}: the $MPC_{hh\ food, water}$ of 0.062 $\mu g.L^{-1}$. The MPC_{marine} is also determined by the $MPC_{hh\ food, water}$: 0.062 $\mu g.L^{-1}$.

3.3.4 $MPC_{dw, water}$

No A1 value and DW standard are available for 1,3-butadiene. With the oral limit value of 0.01 $\mu g.kg_{bw}^{-1}.d^{-1}$ an $MPC_{dw, water, provisional}$ can be calculated with the following formula: $MPC_{dw, water, provisional} = 0.1.TL_{hh}.BW / Uptake_{dw}$ where TL_{hh} is the oral limit value, BW is a body weight of 70 kg, and $uptake_{dw}$ is a daily uptake of 2 L. As described in section 2.2 water treatment is currently not taken into account. Therefore the $MPC_{dw, water} = MPC_{dw,water, provisional}$ and becomes: 0.1 x 0.01 x 70 / 2 = 0.035 $\mu g.L^{-1}$.

3.3.5 Derivation of MAC_{eco}

In the RAR the $PNEC_{water}$ is based on a QSAR dataset. We will also base the $MAC_{eco, water}$ on this same dataset (Table 7). Since for the $PNEC_{water}$ the highest assessment factor was applied, we will also apply the highest assessment factor for compounds which have no potential to bioaccumulate. This factor is 100. The $MAC_{eco, water}$ will be: 32.6 / 100 = 0.33 $mg.L^{-1}$.

There is no data for additional marine taxonomic groups. Therefore, the $MAC_{eco, marine}$ is derived with an additional assessment factor of 10 on 0.33 / 10 = 0.033 $mg.L^{-1}$. It has to be noted that this procedure for the $MAC_{eco, marine}$ is currently not agreed upon. Therefore the $MAC_{eco, marine}$ needs to be re-evaluated once an agreed procedure is available.

3.3.6 Derivation of NC

The NC_{water} is set a factor 100 lower than the MPC_{water}: 0.62 $ng.L^{-1}$.
The NC_{marine} is set a factor 100 lower than the MPC_{marine}: 0.62 $ng.L^{-1}$.

3.3.7 Derivation of $SRC_{eco, aquatic}$

To calculate an $SRC_{eco, aquatic}$, the same QSAR derived dataset as used in the RAR to derive the PNEC has been used (Table 7). The geometric mean of the acute values divided by 10 (3.7 $mg.L^{-1}$) is lower than the geometric mean of the chronic values (5.2 $mg.L^{-1}$). Therefore the $SRC_{eco, aquatic}$ is derived from the acute data: 3.7 $mg.L^{-1}$. The $SRC_{eco, aquatic}$ is valid for the marine and the freshwater environment.

3.4 Toxicity data and derivation of ERLs for sediment

The log $K_{p, susp-water}$ of 1,3-butadiene is below the trigger value of 3, therefore, ERLs are not derived for sediment.

3.5 Toxicity data and derivation of ERLs for soil

No data is presented in the RAR for soil toxicity.

3.5.1 Derivation of MPC_{soil}

3.5.1.1 $MPC_{eco, soil}$

The $PNEC_{soil}$ derived in the RAR was calculated from the $PNEC_{water}$ using equilibrium partitioning. The derived value is 45.6 $\mu g.kg_{ww}^{-1}$. Recalculation to dry weight standard Dutch soil gives: 151.6 $\mu g.kg_{dwt}^{-1}$. This value will be taken over as $MPC_{eco, soil}$: 151.6 $\mu g.kg_{dwt}^{-1}$ for Dutch standard soil.

3.5.1.2 $MPC_{sp, soil}$

1,3-Butadiene has a log $K_{ow} < 3$ and therefore secondary poisoning is not triggered.

3.5.1.3 $MPC_{human, soil}$

For the derivation of the $MPC_{human, soil}$, the oral limit value of 0.01 $\mu g.kg_{bw}^{-1}.day^{-1}$ can be used as TL_{hh} to calculate the $MPC_{human, soil}$ with the method as described in van Vlaardingen and Verbruggen (2007). Specific human intake routes are allowed to contribute 10% of the human toxicological threshold limit. Four different routes contributing to human exposure have been incorporated: consumption of leafy crops, root crops, milk and meat. Uptake via root crops was determined to be the critical route. The calculated $MPC_{human, soil}$ is 0.36 $\mu g.kg_{dwt}^{-1}$ for Dutch standard soil.

3.5.1.4 Selection of the MPC_{soil}

The MPC_{soil} is set by the $MPC_{human, soil}$ at: 0.36 $\mu g.kg_{dwt}^{-1}$.

3.5.2 Derivation of NC_{soil}

The NC_{soil} is set a factor 100 lower than the MPC_{soil}: 3.6 $ng.kg_{dwt}^{-1}$.

3.5.3 Derivation of $SRC_{eco, soil}$

The $SRC_{eco, soil}$ can be calculated from the $SRC_{eco, water}$ with equilibrium partitioning: 17 $mg.kg_{dwt}^{-1}$ for Dutch standard soil.

3.6 Derivation of ERLs for groundwater

3.6.1 Derivation of MPC_{gw}

3.6.1.1 $MPC_{eco, gw}$

Since groundwater-specific ecotoxicological ERLs for the groundwater compartment are absent, the surface water $MPC_{eco, water}$ is taken as substitute. Thus, $MPC_{eco, gw} = MPC_{eco, water} = 32.6\ \mu g.L^{-1}$.

3.6.2 $MPC_{human, gw}$

The $MPC_{human, gw}$ is set equal to the $MPC_{dw, water}$ of 0.035 $\mu g.L^{-1}$. Therefore the $MPC_{human, gw} = MPC_{dw, water}$: 0.035 $\mu g.L^{-1}$.

3.6.3 Selection of the MPC_{gw}

The lowest available MPC is the $MPC_{human, gw}$ of 0.035 $\mu g.L^{-1}$. Thus, the final $MPC_{gw} = 0.035\ \mu g.L^{-1}$.

3.6.4 Derivation of NC_{gw}

The NC_{gw} is set a factor 100 lower than the MPC_{gw}. Thus, NC_{gw} is 0.35 $ng.L^{-1}$.

3.6.5 Derivation of $SRC_{eco, gw}$

The $SRC_{eco, gw}$ is set equal to $SRC_{eco, aquatic}$. Thus, the $SRC_{eco, gw} = 3.7\ mg.L^{-1}$.

3.7 Derivation of ERLs for air

Ecotoxicological data for the air compartment are reported in Table 9.

Table 9. 1,3-Butadiene: selected air data for ERL derivation

Chronic		**Acute**	
Taxonomic group	**NOEC ($mg.m^{-3}$)**	**Taxonomic group**	**L(E)C_{50} ($g.m^{-3}$)**
Plants		**Plants**	
Gossypium hirsutum	22.1 (21 days)	*Pisum sativum*	1.110×10^{6} (3 h)*
Vigna sinensis	2210 (7 days)	*Phaseolus vulgaris*	2.22×10^{4} (4 h)*
Lycopersicum esculentum	22.1 (21 days)		
Coleus spec.	22.1 (21 days)		
Sorghum spec.	2210 (7 days)		
Glycine soja	2210 (7 days)		

Chronic Taxonomic group	NOEC ($mg.m^{-3}$)	Acute Taxonomic group	$L(E)C_{50}$ ($g.m^{-3}$)
Mammals			
mice (NOAEL/LOAEL)	13.8 (2 year)		

* effect possibly due to traces of ethylene.

3.7.1 Derivation of MPC_{air}

3.7.1.1 $MPC_{eco, air}$

In the RAR a $PNEC_{air}$ for plants is derived of 2.2 $mg.m^{-3}$ using an assessment factor of 10 on the NOECs of 22.1 $mg.m^{-3}$ for 21 days exposure. This assessment factor was applied since other plant species exposed to 100 times higher concentrations showed no effect. From the mammalian data a $PNEC_{air}$ was derived of 1.38 $mg.m^{-3}$ using an assessment factor of 10. Both PNECs are similar and, in the RAR, no selection is made for a final $PNEC_{air}$. However the plant PNEC is used in the risk assessment and therefore this one is also selected as the $MPC_{eco, air}$: 2.2 $mg.m^{-3}$.

3.7.1.2 Derivation of $MPC_{human, air}$

The $MPC_{human, air}$ will be equal to the TCA as given in section 3.1.5. The $MPC_{human, air}$ is: 0.03 $\mu g.m^{-3}$.

3.7.1.3 Selection of the MPC_{air}

The MPC_{air} will be the lowest MPC_{air}, the $MPC_{human, air}$ of: 0.03 $\mu g.m^{-3}$.

3.7.2 Derivation of NC_{air}

The MPC_{air} divided by 100 is the NC_{air}: 0.3 $ng.m^{-3}$.

3.8 Comparison of derived ERLs with monitoring data

The RIWA (Dutch Association of River Water companies, www.riwa.org) reports no monitoring data for 1,3-butadiene between 2001 and 2006. Also the Dutch Ministry of Transport, Public Works and Water Management does not present any monitoring data for 1,3-butadiene on their website (www.waterstat.nl). According to the RAR only two reports mentioning 1,3-butadiene in surface water are available. The first report mentions a concentration of 2 $\mu g.L^{-1}$ in the San Francisco Bay area in the USA in 1975-76. The second report mentions detection of 1,3-butadiene in 2 out of 2103 samples in the effluent from a production plant in Canada in 1996. The levels in the two samples were 2 $\mu g.L^{-1}$and 5 $\mu g.L^{-1}$, these levels would have been further diluted in the receiving water. Comparison to the derived MPC_{water} of 0.062 $\mu g.L^{-1}$ shows that these observations would have exceeded the MPC_{water} derived in this report. The MAC_{eco} and SRC_{eco} derived in this report would not have been exceeded.

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 1,3-butadiene in water, groundwater, soil and air. No risk limits were derived for the sediment compartment, because exposure of sediment is considered negligible. It should be noted that because of the physical nature of the substance, the derived ERLs are based on QSAR calculated aquatic toxicity data. Due to its high vapour pressure and flammable nature it would be very difficult to test meaningfully. Because of this reason there is a higher uncertainty in the derived ERLs than when experimentally derived aquatic toxicity data are used. The ERLs that were obtained are summarised in the table below. Monitoring data for 1,3-butadiene in the Dutch environment are not available. Therefore it cannot be judged if the derived ERLs are being exceeded.

Table 10. Derived MPC, NC, MAC_{eco}, and SRC_{eco} values for 1,3-butadiene.

ERL	**unit**	**value**			
		MPC	NC	MAC_{eco}	SRC_{eco}
water [a]	$ng.L^{-1}$	62	0.62	3.3×10^{5} [d]	3.7×10^{6} [d]
drinking water [b]	$ng.L^{-1}$	35			
marine	$ng.L^{-1}$	62	0.62	3.3×10^{4} [d]	3.7×10^{6} [d]
sediment	$mg.kg_{dwt}^{-1}$	n.d.			
soil [c]	$\mu g.kg_{dwt}^{-1}$	0.36	3.6×10^{-3}		1.7×10^{4} [e]
groundwater	$ng.L^{-1}$	35	0.35		3.7×10^{6} [d]
air	$ng.m^{-3}$	30	0.30		

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

[b] The exact way of implementation of the $MPC_{dw, water}$ in the Netherlands is at present under discussion. Therefore, the $MPC_{dw, water}$ is presented as a separate value in this report.

[c] Expressed on the basis of Dutch standard soil.

[d] Value based on QSARs for toxicity.

[e] Value based on QSARs for toxicity and equilibrium partitioning.

n.d. = not derived.

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