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Rapport in het kort

Milieurisicogrenzen voor DODMAC en DHTDMAC

Dit rapport geeft milieurisicogrenzen voor de totale concentratie van DODMAC (dimethyldioctadecylammonium chloride) en DHTDMAC (di(geharde talk)dimethylammoniumchloride) in (grond)water, bodem en sediment. Milieurisicogrenzen zijn de technisch-wetenschappelijke advieswaarden voor de uiteindelijke milieukwaliteitsnormen in Nederland. Deze milieurisicogrenzen zijn gebaseerd op de uitkomsten van de EU risicobeoordeling voor DODMAC (Bestaande Stoffen Verordening 793/93). De afleiding van de milieurisicogrenzen sluit tevens aan bij de richtlijnen uit de Kaderrichtlijn Water. De laatst beschikbare monitoringsgegevens voor oppervlakte water uit 1990 overschrijden de afgeleide milieurisicogrens. Vanwege onvoldoende informatie over de huidige productievolumes en het hedendaags gebruik van DODMAC kan niet worden ingeschat of de afgeleide milieurisicogrenzen ook nu nog overschreden worden.

Trefwoorden: milieurisicogrenzen; DODMAC; dimethyldioctadecylammonium chloride; 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 the total concentration of DODMAC and DHTDMAC in water, groundwater, sediment and soil. The combined presence of DODMAC and DHTDMAC is reason to consider both compounds together for ERL-derivation. 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 for the air compartment were derived (not relevant). The NC protects for human and environmental exposure to several substances at the same time (mixture toxicity).

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.

Since there is only monitoring data for DODMAC/DHTDMAC from the past and considering uncertainties in the current consumption and use of DODMAC it cannot be estimated whether the derived ERLs are currently exceeded in the Dutch environment. Therefore, environmental monitoring of this compound may be considered.

Table 1. Derived MPC, NC, MAC_{eco}, and SRC_{eco} values for the total concentration of DODMAC and DHTDMAC.

ERL	**unit**	**value**			
		MPC	NC	MAC_{eco}	SRC_{eco}
water [a]	$\mu g.L^{-1}$	6.2	6.2×10^{-2}	6.2	1.1×10^{2}
water susp. matter	$mg.kg_{dwt}^{-1}$	77			
drinking water [b]	$\mu g.L^{-1}$	6.0×10^{2}			
marine	$\mu g.L^{-1}$	0.62	6.2×10^{-3}	0.62	1.1×10^{2}
marine susp. matter	$mg.kg_{dwt}^{-1}$	12			
sediment	$mg.kg_{dwt}^{-1}$	55	0.55	n.a.	1.4×10^{3}
marine sediment	$mg.kg_{dwt}^{-1}$	11	0.11	n.a.	1.4×10^{3}
soil	$mg.kg_{dwt}^{-1}$	20 [c]	0.20	n.a.	3.0×10^{2}
groundwater	$\mu g.L^{-1}$	6.2	6.2×10^{-2}	n.a.	1.1×10^{2}
air	$\mu g.m^{-3}$	n.a.			

[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 $MPC_{dw, water}$ is presented as a separate value in this report.

[c] The MPC_{soil} is based on the $MPC_{eco, soil}$ because human exposure through food consumption is considered not realistic.

n.a. = not applicable.

1 Introduction

1.1 Project framework

In this report environmental risk limits (ERLs) for surface water (freshwater and marine), sediment, soil and groundwater are derived for DODMAC. 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 DODMAC

The Risk Assessment Report (RAR) (European Commission, 2002) reports that dimethyldioctadecylammonium chloride (DODMAC) is not produced as an isolated substance or used in a commercial range. DODMAC occurs as a major component of the technical product dihydrogenated tallow dimethylammonium chloride (DHTDMAC). The proportion of DODMAC is about 42% related to the total content of dialkyldimethylammonium compounds. The combined presence of DODMAC and DHTDMAC is reason to consider both compounds together for ERL-derivation (see Section 3.3). The actual production volume in Europe was estimated at 5,004 t in 1996 and 5,651 t in 1997. DHTDMAC is mainly used in the EU in fabric softeners, car washing agents and hair conditioners and for the synthesis of organic clay. More information can be found in the RAR (European Commission, 2002). DODMAC is also discussed in the PBT working group of the EU Technical Committee on new and existing substances in the context of another product than mentioned above. This suggests that there are more and new applications for DODMAC and the production and use in Europe might be higher than estimated in the RAR.

2 Methods

2.1 Data collection

The final Risk Assessment Report (RAR) of DODMAC (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 peer-reviewed by the Scientific Committee on Toxicity, Ecotoxicity and the Environment (CSTEE). In their opinion, the CSTEE endorses the conclusion in the RAR. 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. Considering the salty character of DODMAC, however, no ERLs for air are derived.

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 $MPC_{dw, water}$ 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.

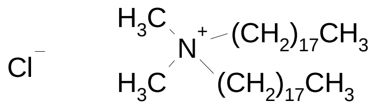
If freshwater and marine data sets are not combined the $MAC_{eco,\ marine}$ is derived on the marine toxicity data using the same additional assessment factors as mentioned above. It has to be noted that this procedure is currently not formalised. Therefore, the $MAC_{eco,\ marine}$ value needs to be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

3 Derivation of environmental risk limits for DODMAC + DHTDMAC

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

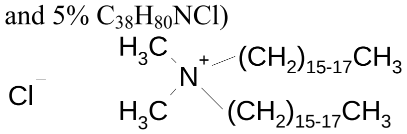
3.1.1 Identity

Table 2. Identification of DODMAC.

Parameter	Name or number
Chemical name	dimethyldioctadecylammonium chloride
Common/trivial/other name	DODMAC, Distearyldimethylammonium chloride (DSDMAC)
CAS number	107-64-2
EC number	203-508-2
Molecular formula	$C_{38}H_{80}NCl$
Structural formula	

DODMAC is only produced in the technical product ditallowdimethylammonium chloride (DHTDMAC). In the RAR the content of DODMAC in DHTDMAC is estimated at 42%.

Table 3. Identification of DHTDMAC.

Parameter	Name or number
Chemical name	ditallowdimethylammonium chloride
Common/trivial/other name	DHTDMAC, di(hydrogenated tallow alkyl) dimethylammoniumchlorides
CAS number	61789-80-8
EC number	263-090-2
Molecular formula	$C_{36.4}H_{76.8}NCl$ (related to approx. 65% $C_{38}H_{80}NCl$, 30% $C_{34}H_{72}NCl$ and 5% $C_{38}H_{80}NCl$)
Structural formula	

3.1.2 Physico-chemical properties

Table 4. Physico-chemical properties of DODMAC.

Parameter	Unit	Value	Remark
Molecular weight	[g.mol^{-1}]	586.52	DODMAC
Water solubility	[pg.L^{-1}]	< 1	also reported as not soluble but dispersible up to 2.7 mg.L^{-1}
log K_{OW}	[-]	3.80	The reliability of this value is questionable since it is a surface active compound and in solution always present in the dissociated form. The K_{ow} should be determined on non-dissociated compounds.
K_{OC}	[L.kg^{-1}]	n.a.	not derived, see section 3.1.3
$K_{p\ susp\text{-}water}$	[L.kg^{-1}]	16 800	value calculated in the RAR from adsorption of DHTDMAC on sediment
Vapour pressure	[Pa]	-	negligible because of the salt character. In the RAR an estimated value of 10^{-15} Pa is used.
Melting point	[°C]	72-122	
Boiling point	[°C]	-	decomposes at 135°C
Henry's law constant	[Pa.m^3.mol^{-1}]	n.a.	

n.a. = not applicable.

In the RAR is stated that both DODMAC and DHTDMAC have to be considered as nearly insoluble in water. However, the compound does form stable dispersions in water. All relevant concentrations in the environment, wastewater or toxicity test solutions are far above the water solubility. It is evident that in the hydrosphere DODMAC (and DHTDMAC) is not really dissolved but always adsorbed onto suspended matter or included in vesicles together with other lipophilic organics (e.g. humic acids, tensides). The water solubility is not a limiting factor for emissions into wastewater or pollution of the hydrosphere. Therefore, all test solutions with concentrations up to the maximum dispersibility are considered acceptable for the toxicity tests.

3.1.3 Behaviour in the environment

Table 5. Selected environmental properties of DODMAC.

Parameter	Unit	Value	Remark
Hydrolysis half-life	DT50 [d]	n.a.	
Photolysis half-life	DT50 [d]	n.a.	
Degradability			not readily degradable

n.a. = not available

As revealed by investigations reported in the EU-RAR, DODMAC adsorbs onto both the mineral and the organic fraction of soil and sediments. Therefore, the determination of a K_{oc} from log K_{ow} is not opportune, because the common K_{oc} derivations are not valid for surface active substances like DODMAC. In the EU-RAR the value of 10000 L.kg^{-1} is used for both the Kp_{soil} and Kp_{sed}.

3.1.4 Bioconcentration and biomagnification

An overview of the bioaccumulation data for DODMAC is given in Table 6.

Table 6. Overview of bioaccumulation data for DODMAC.

Parameter	Unit	Value	Remark
BCF (fish)	[$L.kg^{-1}$]	< 2000	estimated value based on measured concentrations, used in the RAR risk assessments.
BMF	[$kg.kg^{-1}$]	1	default value since the BCF <2000 $L.kg^{-1}$.

In the RAR an estimated value of 13 $L.kg^{-1}$ based on measured concentrations is used. However, considering the poor solubility and characteristics of DODMAC, it is questionable if the compound is actually taken up into the body or actually sorbed to the skin of the fish. In laboratory tests the substance is most likely to absorb to the mucus and uptake of DODMAC into the body will proceed through the food rather than through water. Therefore, the PBT working group of the EU Technical Committee on new and existing substances in their meeting on 6 November 2006 determined this BCF to be unreliable and stated that it should be higher than 13 $L.kg^{-1}$. Later, the RIVM has submitted evidence for the BCF to be < 2000 $L.kg^{-1}$. This value is used in this report. If a more precise value would be required, additional tests would be necessary.

3.1.5 Human toxicological threshold limits and carcinogenicity

Classification and labelling according to the 25^{th} ATP of Directive 67/548/EEC:
Classification: R41, 50/53. Labelling: Xi (irritant), N (dangerous for the environment)
In the RAR an oral NOAEL of 100 $mg.kg_{bw}^{-1}.day^{-1}$ is used. This NOAEL is based on a 28 day repeated dose rat study. RIVM-SIR has derived an oral limit value of 170 $\mu g.kg_{bw}^{-1}.day^{-1}$ by applying an assessment factor of 600. The assessment factor consists of an interspecies factor of 10, an intraspecies factor of 10 and a factor of 6 because it concerns a sub-acute toxicity study.

3.2 Trigger values

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

Table 7. DODMAC: collected properties for comparison to MPC triggers.

Parameter	Value	Unit	Method/Source
Log $K_{p,susp-water}$	4.2	[-]	value calculated in the RAR from adsorption of DHTDMAC on sediment
BCF	< 2000	[$L.kg^{-1}$]	
BMF	1	[$kg.kg^{-1}$]	
Log K_{OW}	3.8	[-]	
R-phrases	R34, 41, 50/53	[-]	
A1 value	-	[$\mu g.L^{-1}$]	
DW standard	-	[$\mu g.L^{-1}$]	

- DODMAC has a log $K_{p, susp-water}$ > 3; derivation of $MPC_{sediment}$ is triggered.
- DODMAC has a log $K_{p, susp-water}$ > 3; expression of the MPC_{water} as $MPC_{susp, water}$ is required.
- DODMAC has a BCF < 2000 $L.kg^{-1}$; it cannot be concluded that the BCF is < 100 $L.kg^{-1}$, therefore, assessment of secondary poisoning is triggered.
- DODMAC has no R classification for which an MPC_{water} for human health via food (fish) consumption ($MPC_{hh\ food,\ water}$) should be derived.

The BCF of DODMAC was set at < 2000 L.kg^{-1}. However, bioaccumulation of DODMAC is not likely since the Maximum Molecular Length of DODMAC is 4.7 nm. This value is higher than 4.3 nm which is given in the REACH guidance for PBT assessment (ECHA, 2008) as the limit above which bioaccumulation should not occur. Therefore, it can be assumed that it is not likely that the BCF will be higher than 1000 L.kg^{-1}.

3.3 Toxicity data and derivation of ERLs for water

An overview of the selected freshwater toxicity data for DODMAC as reported in the RAR is given in

Table 8 and marine toxicity data are shown in Table 9. Not only data for DODMAC are given. The RAR states that “because the data basis for the pure DODMAC (> 95% purity, C18-chain length) would be too small to reveal all these parameters, it is necessary to use ecotoxicological test results for the commercial product DHTDMAC (71-78% active ingredient = quarternary ammonia, different chain lengths) for the effects assessment”. In the RAR the toxicity data for DHTDMAC are used as they would be for DODMAC and are not corrected for the fraction of DODMAC in DHTDMAC. In this report the same approach is used. The RAR also reports values for DHTDMAC containing another co-substrate, MTTMAC, these values have not been taken into account. Since the toxicity data is based on DHTDMAC and DODMAC both and DODMAC is only produced in as part of DHTDMAC, the ERLs derived are for the total concentration of DODMAC and DHTDMAC together.
It has to be noted that in the RAR species specific data have not been averaged for derivation of the PNEC. Since data with the same endpoint should be averaged (van Vlaardingen and Verbruggen, 2007) this has been done so in the footnote of Table 7. In some cases there is a high difference between the toxicity values for one species presented in the RAR. From the limited information in the RAR this difference seems to be explained by the different test water used, i.e. laboratory water vs. natural water. It is however not the case that the one type of test water always gives lower test results than the other. In some cases, the values in table 7 show lower EC50 values than NOEC values. No explanation for these events are given in the RAR, the best explanations are differences in test set-ups like the test water used and exposure time. However not enough test details are given in the RAR to examine these differences in detail.

Table 8. DODMAC/DHTDMAC: selected freshwater toxicity data for ERL derivation.

Chronic Taxonomic group	$NOEC/EC_{10}$ ($mg.L^{-1}$)	Acute Taxonomic group	$L(E)C_{50}$ ($mg.L^{-1}$)
		Bacteria	
		Pseudomonas putida [a]	53 [g]
Algae		**Algae**	
Pseudokirchneriella subcapitata [a]	**0.062** [c]	*Pseudokirchneriella subcapitata* [b]	0.014 [h]
Microcystis aeruginosa [a]	0.1 [d]	*Microcystis aeruginosa*	0.05
Crustacea		**Crustacea**	
Daphnia magna [b]	0.26 [e]	*Ceriodaphnia dubia* [b]	0.74 [i]
		Daphnia magna [b]	0.016 [j]
Pisces		**Pisces**	
Pimephales promelas [a]	0.11 [f]	*Lepomis macrochirus* [b]	0.62 [k]
		Pimephales promelas [b]	0.29 [l]

[a] Tested substance: DHTDMAC.

[b] Tested substance: DODMAC and DHTDMAC

[c] The geometric mean of all data for *P. subcapitata* with the same exposure time is 0.07 $mg.L^{-1}$. This is based on the two values 0.078 and **0.062** $mg.L^{-1}$.

[d] Geometric mean of 0.13 and 0.078 $mg.L^{-1}$

[e] Geometric mean of 0.38 and 0.18 $mg.L^{-1}$

[f] Geometric mean of 0.053 and 0.23 $mg.L^{-1}$

[g] Geometric mean of 48 and 58 $mg.L^{-1}$

[h] Lowest EC50 values since values differ by a factor 84

[i] Geometric mean of 0.070 and 0.078 $mg.L^{-1}$

[j] Lowest LC50 values since values differ by a factor 19

[k] Lowest LC50 values since values differ by a factor 16

[l] Lowest LC50 values since values differ by a factor 73

The **bold** value is used for MPC derivation

Table 9. DODMAC: selected marine toxicity data for ERL derivation.

Chronic Taxonomic group	$NOEC/EC_{10}$ ($mg.L^{-1}$)	Acute Taxonomic group	$L(E)C_{50}$ ($mg.L^{-1}$)
Crustacea		**Crustacea**	
Mysidopsis bahia [a]	0.075	*Mysidopsis bahia* [a]	0.22

[a] Tested substance: DHTDMAC

3.3.1 Treatment of fresh- and marine water toxicity data

In the RAR no separate PNEC value for the marine environment has been derived. Toxicity data are presented for only one marine species giving an incomplete dataset for the marine environment. It is also mentioned that there are no large differences in the range of toxicity between marine/estuarine and limnic species. Therefore data for freshwater and marine species are pooled.

3.3.2 Mesocosm studies

No mesocosm studies are reported 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 a $PNEC_{water}$ of 6.2 $\mu g.L^{-1}$ has been derived for the aquatic compartment. The key value for this derivation was an individual NOEC of 62 $\mu g.L^{-1}$ for DHTDMAC for *Pseudokirchneriella subcapitata*. In the RAR, no reason was given why the lowest value was selected and not the geometric mean of the two values available for *P. subcapitata*. Despite this, the $MPC_{eco, water}$ will be set equal to the $PNEC_{water}$ from the RAR at: 6.2 $\mu g.L^{-1}$.
In the RAR no separate $PNEC_{marine}$ has been derived. Following the TGD and using the same dataset and reasoning a factor of 100 should be applied to the used NOEC of 62 $\mu g.L^{-1}$ for DHTDMAC for *P. subcapitata*. The $MPC_{eco, marine}$ is: 0.62 $\mu g.L^{-1}$.

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

DODMAC has a BCF potentially > 100 $L.kg^{-1}$, therefore assessment of secondary poisoning is triggered. The MPC_{oral} per species is calculated applying the appropriate assessment factor (see Table 10). The lowest value is used for MPC derivation according to Eq. 13 of the INS-Guidance.

Table 10. DODMAC: toxicity data for birds and mammals.

Species	Exposure time	Criterion	Effect concentration ($mg.kg_{diet}^{-1}$)	Assessment factor	MPC_{oral} ($mg.kg_{diet}^{-1}$)
Rat	28 days	NOEC	2000	300	6.67
Rat	28 days	NOEC	2500	300	8.33

The NOECs reported above have been calculated in the RAR from chronic NOAELs of 100 and 125 $mg.kg_{bw}^{-1}.day^{-1}$ for rats for repeated oral dose toxicity and reproductive toxicity respectively. As reported in Van Vlaardingen and Verbruggen (2007) these values can be converted into a NOEC in $mg.kg_{diet}^{-1}$ using a conversion factor of 20. With an assessment factor of 300 as used for short term exposed mammals, the $MPCs_{oral}$ are calculated. The lowest one will be used to calculate the $MPC_{sp, water}$ and $MPC_{sp, marine}$. Since there is no unbound BCF value, it is examined at which BCF the $MPC_{sp, water}$ will be equal to the $MPC_{eco, water}$. This is at a BCF of 6.67 / 0.0062 = 1076 $L.kg^{-1}$. Nevertheless, bioaccumulation of DODMAC is not likely since the Maximum Molecular Length of DODMAC is 4.7 nm. This value is higher than 4.3 nm which is given in the REACH guidance for PBT assessment (ECHA, 2008) as the limit above which bioaccumulation is not expected to occur. Therefore, it can be assumed that the $MPC_{sp, water}$ will be higher than the $MPC_{eco, water}$.

The $MPC_{sp, marine}$ with a maximum BCF of 2000 is 3.3 $\mu g.L^{-1}$, this value is higher than the $MPC_{eco, marine}$.

3.3.3.3 $MPC_{hh food, water}$

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

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

The lowest MPC_{water} is the $MPC_{eco, water}$ of 6.2 $\mu g.L^{-1}$ [1].
The lowest MPC_{marine} is the $MPC_{eco, marine}$ of 0.62 $\mu g.L^{-1}$ [2].

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[1] The MPC_{water} reflects the total concentration of DODMAC and DHTDMAC together.

[2] The MPC_{marine} reflects the total concentration of DODMAC and DHTDMAC together.

DODMAC has a log $K_{p,\ susp\text{-}water} \geq 3$; expression of the MPC_{water} as $MPC_{susp,\ water}$ is required. The $MPC_{susp,\ water}$ is calculated according to:

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

For this calculation, $K_{p,susp\text{-}water,Dutch\ standard}$ is calculated from the $K_{p,\ susp\text{-}water}$ of 16800 $L.kg^{-1}$ as calculated in the RAR based on a $f_{OC,susp}$ of 0.1. With an $f_{OC,susp,\ Dutch\ standard}$ of 0.1176 the $K_{p,\ susp\text{-}water,\ Dutch\ standard}$ can be recalculated to 19757 $L.kg^{-1}$. With this value and a $C_{susp,\ Dutch\ standard}$ of 30 $mg.L^{-1}$ the $MPC_{susp,\ water}$ is: 76.9 $mg.kg_{dwt}^{-1}$.

The $MPC_{susp,\ marine}$ is calculated in a similar way from the MPC_{marine} and a $C_{susp,\ marine}$ of 3 $mg.L^{-1}$ at: 11.6 $mg.kg_{dwt}^{-1}$.

3.3.4 Derivation of $MPC_{dw,\ water}$

No A1 value and DW standard are available for DODMAC. With the ADI (oral limit value, derived in paragraph 3.1.5) of 170 $\mu g.kg_{bw}^{-1}day^{-1}$ an $MPC_{dw,\ water,\ provisional}$ can be calculated with the following formula: $MPC_{dw,\ water,\ provisional} = 0.1.TL_{hh}.BW / uptake_{dw}$ where the TL_{hh} is the TDI, 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 $MPC_{dw,\ water}$ = The $MPC_{dw,water,\ provisional}$ and becomes: 0.1 * 170 * 70 / 2 = 595 $\mu g.L^{-1}$.

3.3.5 Derivation of MAC_{eco}

In the RAR the lowest L/EC50-value reported is 0.014 $mg.L^{-1}$ for *Pseudokirchneriella subcapitata*. DODMAC has no potential to bioaccumulate, but the acute toxicity data differ by more than a factor of 3, this results in an assessment factor of 100. The $MAC_{eco,\ water}$ is initially set to: 0.014 / 100 = 0.14 $\mu g.L^{-1}$. This value is lower than the $MPC_{eco,\ water}$ of 6.2 $\mu g.L^{-1}$. This value is not deemed realistic since this would imply that one expects acute toxic effects at concentrations below the ERL that protects from chronic exposure (van Vlaardingen and Verbruggen 2007). In the RAR no explanation is given for this fact but it is probably an artefact caused by the high variety of acute values for *Pseudokirchneriella subcapitata*. Therefore, the $MAC_{eco,\ water}$ is set equal to the $MPC_{eco,\ water}$: 6.2 $\mu g.L^{-1}$. The $MAC_{eco,\ marine}$ is set a factor of 10 lower than the $MAC_{eco,\ water}$ because there is no acute toxicity data for additional marine taxonomic groups. The crustacean in Table 8 does not account as an additional marine taxonomic group since it has the same life form and feeding strategy as freshwater crustacea like *Daphnia* sp. The $MAC_{eco,\ marine}$ is initially set to 0.014 / 100 / 10 = 0.014 $\mu g.L^{-1}$. Since this value is lower than the $MPC_{eco,\ marine}$ of 0.62 $\mu g.L^{-1}$, the $MAC_{eco,\ marine}$ is set equal to the $MPC_{eco,\ marine}$: 0.62 $\mu g.L^{-1}$. It has to be noted that this procedure for $MAC_{eco,\ marine}$ 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} and NC_{marine} are set a factor of 100 lower than the final MPC. The NC_{water} is: 0.062 $\mu g.L^{-1}$; the MPC_{marine} is 0.0062 $\mu g.L^{-1}$.

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

As presented in Table 7 and 8, chronic and acute data are available for three and four taxa respectively. The base set of chronic data for three taxa (algae, *Daphnia* and fish) is present, therefore the $SRC_{eco,\ aquatic}$ is based on the geometric mean of all chronic values: 0.11 $mg.L^{-1}$. The $SRC_{eco,\ aquatic}$ is valid for the marine and the freshwater environment.

3.4 Toxicity data and derivation of ERLs for sediment

An overview of the freshwater sediment toxicity data reported in the RAR for DODMAC and DHTDMAC is given in Table 9. Data for marine sediments are not reported in the RAR. Not only data for DODMAC are given. The RAR states that “because the data basis for the pure DODMAC (> 95% purity, C18-chain length) would be too small to reveal all these parameters, it is necessary to use ecotoxicological test results for the commercial product DHTDMAC (containing about 42% DODMAC and for the rest other quaternary ammonium compounds with alkyl chains with a length ranging from C_{12} to C_{20}) for the effects assessment”. Since the toxicity data is based on DHTDMAC and DODMAC both and DODMAC is only produced in as part of DHTDMAC, the ERLs derived are for the total concentration of DODMAC and DHTDMAC together.

Table 11. DODMAC: selected freshwater sediment toxicity data for ERL derivation.

Chronic **Taxonomic group**	**NOEC/EC10 (mg.kg$_{dwt}^{-1}$)**	**Acute** **Taxonomic group**	**L(E)C50**
Nematoda			
Caenorhabditis elegans	1350 [a]		
Annelida			
Lumbriculus variegatus	5000		
Tubifex tubifex	**550**		
Insecta			
Chironomus riparius	876		

Bold value is used for derivation of the MPC.
[a] DHTDMAC

3.4.1 Derivation of MPC$_{sediment}$

In the RAR the EC10 of 550 mg.kg$_{dwt}^{-1}$ for *Tubifex tubifex* is used with an assessment factor of 10 to derive a PNEC$_{sediment}$: 55 mg.kg$_{dwt}^{-1}$. The MPC$_{sediment}$ is set equal to the PNEC$_{sediment}$: 55 mg.kg$_{dwt}^{-1}$.

No data for marine sediment species are presented in the RAR. However, with three long term sediment tests with freshwater species representing different living and feeding conditions, the same EC10 can be used with an assessment factor of 50. The MPC$_{marine\ sediment}$ is 550/50 = 11 mg.kg$_{dwt}^{-1}$.

In the EU-RAR no conversion to a standard sediment is performed since the bioavailability of DODMAC and DHTDMAC are not determined by the organic content alone. Therefore the MPC$_{sediment}$ derived are not converted to Dutch standard sediment.

3.4.2 Derivation of NC$_{sediment}$

The NC is set a factor 100 lower than the MPC. The NC$_{sediment}$ is: 0.55 mg.kg$_{dwt}^{-1}$. The NC$_{marine\ sediment}$ is: 0.11 mg.kg$_{dwt}^{-1}$.

3.4.3 Derivation of SRC$_{eco,\ sediment}$

Only NOECs are available in the RAR, therefore the SRC$_{eco,\ sediment}$ is geometric mean of all NOECs in Table 9: 1376 mg.kg$_{dwt}^{-1}$.

3.5 Toxicity data and derivation of ERLs for soil

An overview of the soil toxicity data for DODMAC/DHTDMAC as presented in the RAR is given in Table 12. Because there were no terrestrial data for DODMAC itself, only results for DHTDMAC are given in the RAR. In the RAR is also stated that "so far there is no proof that the toxicity of both substances varies significantly". Since the toxicity data is based on DHTDMAC both and DODMAC is only produced in as part of DHTDMAC, the ERLs derived are for the total concentration of DODMAC and DHTDMAC together.

Table 12. DODMAC: selected soil data for ERL derivation.

Chronic **Taxonomic group**	**NOEC/EC10 (mg.kg$_{dwt}^{-1}$)**	**Acute** **Taxonomic group**	**L(E)C50 (mg.kg$_{dwt}^{-1}$)**
Bacteria			
soil microorganisms	≥ 400 (14w) [a]		
soil microorganisms	≥ 365 (28d) [a]		
Macrophyta			
Sinapis alba	1400 (EC5) [a]	*Sinapis alba*	3540 [a]
Triticum aestivum	>1000 (EC5) [a]		
Linum utisatissimum	>1000 (EC5) [a]		
Sorghum bicolor	**1000** [a]	*Sorghum bicolor*	2530 [a]
Helianthus annuus	**1000** [a]	*Helianthus annuus*	2930 [a]
Avena sativa	≥1000 [a]		
Brassica rapa	≥1000 [a]		
Lycopersicum esculentum	≥40 000 [a]		
Lactuca sativa	≥40 000 [a]		
Hordeum vulgare	≥40 000 [a]		
Annelida			
Eisenia fetida	≥1000 [a]		

Bold values are used in the derivation of the MPC.

Unbound values (≥) are given as indication and are not used for ERL derivation.

[a] DHTDMAC.

3.5.1 Derivation of MPC_{soil}

3.5.1.1 $MPC_{eco,\ soil}$

In the RAR a $PNEC_{soil}$ of 20 mg.kg$_{dwt}^{-1}$ has been derived using a NOEC of 1000 mg.kg$_{dwt}^{-1}$ and an assessment factor of 50. The assessment factor of 50 is used because it was assumed that two trophic levels are covered with long-term data for plants and micro-organisms. In the EU-RAR is not explained why the endpoint for *Eisenia fetida* is not considered as third trophic level to lower the assessment factor. The $PNEC_{soil}$ is not converted to a standard soil since the bioavailability of DODMAC and DHTDMAC are not determined by the organic content alone. Therefore the $PNEC_{soil}$ is taken over as $MPC_{eco,\ soil}$ and not converted to Dutch standard soil. The $MPC_{eco,\ soil}$ is: 20 mg.kg$_{dwt}^{-1}$.

3.5.1.2 $MPC_{sp,\ soil}$

DODMAC has a log K_{ow} > 3 and therefore secondary poisoning is triggered. However, no valid BCF for earthworms is available and the QSAR given in the INS-guidance is not fully valid because DODMAC is an ionic compound. Therefore it is investigated at which BCF the $MPC_{sp,\ soil}$ would be lower than the $MPC_{eco, soil}$. With a BCF of 2714 $kg_{dwt}.kg_{wwt}^{-1}$, the $MPC_{sp, soil}$ would be equal to the $MPC_{eco, soil}$. This indicates that the BCF should be higher than 2714 $kg_{dwt}.kg^{-1}$ to form an environmental risk through secondary poisoning. To consider whether it would be likely for the BCF to exceed the calculated values the following facts are taken into account: the BCF for fish is considered to be lower than 2000 $L.kg^{-1}$; the QSAR-calculated BCF for earthworms is 77 $kg_{dwt}.kg_{wwt}^{-1}$; and a sediment BSAF for *Lumbriculus variegatus* of 0.28 $kg_{dwt}.kg_{wwt}^{-1}$ is presented in the RAR. On the basis of these facts, it can be presumed that the BCF for earthworms will not exceed the value of 2714 $kg_{dwt}.kg^{-1}$. Therefore can be concluded that exposure via secondary poisoning will not pose a greater risk than exposure directly through soil and derivation of an $MPC_{sp, soil}$ is not necessary.

3.5.1.3 $MPC_{human, soil}$

Derivation of the $MPC_{human, soil}$ is not possible for this compound because no reliable values for K_{ow} and solubility are available. Also, the equilibrium partitioning models on which calculation of the $MPC_{human, soil}$ is based are not suitable for this compound.

3.5.1.4 Selection of the MPC_{soil}

The only MPC_{soil} available is the $MPC_{eco, soil}$. Bioaccumulation of DODMAC is not likely since the Maximum Molecular Length of DODMAC is 4.7 nm. This value is higher than 4.3 nm which is given in the REACH guidance for PBT assessment (ECHA, 2008) as the limit above which bioaccumulation is not expected to occur. Also, the BCF is considered to be < 2000 $kg_{dwt}.kg^{-1}$ and the sediment BSAF for *Lumbriculus variegatus* is 0.28 $kg_{dwt}.kg_{wwt}^{-1}$. Therefore, human exposure to DODMAC through food consumption is not considered realistic. It should also be noted that the $MPC_{hh\ food, water}$ is not triggered either. The exposure via secondary poisoning will not pose a greater risk than exposure directly via soil. Therefore, the MPC_{soil} is set equal to the $MPC_{eco, soil}$: 20 $mg.kg_{dwt}^{-1}$.

3.5.2 Derivation of NC_{soil}

The NC is set a factor 100 lower than the MPC: NC = 0.2 $mg.kg_{dwt}^{-1}$.

3.5.3 Derivation of $SRC_{eco, soil}$

The geometric mean of the NOECs and of the L(E)C50s reported in table 10 have been calculated. Unbounded values (≥) have not been used in this calculation. The geometric mean of the chronic data (1119 $mg.kg_{dwt}^{-1}$) is higher than the geometric mean of the acute data divided by 10 (297 $mg.kg_{dwt}^{-1}$). Therefore the $SRC_{eco, soil}$ will be 297 $mg.kg_{dwt}^{-1}$. Since the bioavailability of DODMAC and DHTDMAC are not determined by the organic content, the $SRC_{eco, soil}$ will not be converted to a 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 a substitute. Thus the $MPC_{eco, gw}$ = $MPC_{eco, water}$ = 6.2 $\mu g.L^{-1}$.

3.6.1.2 $MPC_{human, gw}$

The $MPC_{human, gw}$ is set equal to the $MPC_{dw, water}$. Therefore the $MPC_{human, gw}$ = $MPC_{dw, water}$ = 595 $\mu g.L^{-1}$.

3.6.1.3 Selection of the MPC_{gw}

The lowest MPC_{gw} is the $MPC_{eco, gw}$ of 6.2 $\mu g.L^{-1}$. Thus, the final MPC_{gw} = 6.2 $\mu g.L^{-1}$.

3.6.2 Derivation of NC_{gw}

The NC_{gw} is set a factor 100 lower than the MPC_{gw}: 0.062 $\mu g.L^{-1}$.

3.6.3 Derivation of $SRC_{eco, gw}$

The $SRC_{eco, gw}$ is set equal to the $SRC_{eco, aquatic}$: 110 $\mu g.L^{-1}$.

3.7 Derivation of ERLs for air

No suitable data is presented in the RAR to derive an MPC_{air}. Considering the salty character of DODMAC derivation of an MPC_{air} is not relevant.

3.8 Comparison of derived ERLs with monitoring data

The RIWA (Dutch Association of River Water companies) does not present any monitoring for DODMAC or DHTDMAC in their annual reports between 2001 and 2006. The RAR reports monitoring data for DHTDMAC in Dutch surface water ranging between 15 and 116 $\mu g.L^{-1}$ in 1990 in rivers, canals, tributaries and polders. These values are above the MPC_{water} of 6.2 $\mu g.L^{-1}$ derived in this report. In the RAR a local surface water concentration for the use of DODMAC in fabric softeners, hair conditioners and car washing products is calculated of 8.4 $\mu g.L^{-1}$ for 1989/90 and of 0.42 $\mu g.L^{-1}$ for 1998. This reduction in the PEC is based on the decreased consumption of DHTDMAC between these years. However, since DODMAC is used in more applications than considered in the RAR, the consumption of DODMAC and the environmental concentrations might not be reduced as much as assumed in the RAR. Therefore, the current levels in the Dutch surface water might still exceed the derived ERLs. For other compartments no monitoring data is available.

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 DODMAC in water, groundwater, sediment and soil. The ERLs that were obtained are summarised in Table 13. The ERLs derived are for the total concentration of DODMAC and DHTDMAC together because the toxicity data is based on DHTDMAC and DODMAC both and DODMAC is only produced as part of DHTDMAC. Since there is only monitoring data for DODMAC from the past and considering uncertainties in the current consumption and use of DODMAC it cannot be estimated whether the derived ERLs are currently exceeded in the Dutch environment. Therefore, environmental monitoring of this compound may be considered.

Table 13. Derived MPC, NC, MAC_{eco}, and SRC_{eco} values for the total concentration of DODMAC and DHTDMAC.

ERL	unit	value			
		MPC	NC	MAC_{eco}	SRC_{eco}
water [a]	$\mu g.L^{-1}$	6.2	6.2×10^{-2}	6.2	1.1×10^{2}
water susp. matter	$mg.kg_{dwt}^{-1}$	77			
drinking water [b]	$\mu g.L^{-1}$	6.0×10^{2}			
marine	$\mu g.L^{-1}$	0.62	6.2×10^{-3}	0.62	1.1×10^{2}
marine susp. matter	$mg.kg_{dwt}^{-1}$	12			
sediment	$mg.kg_{dwt}^{-1}$	55	0.55	n.a.	1.4×10^{3}
marine sediment	$mg.kg_{dwt}^{-1}$	11	0.11	n.a.	1.4×10^{3}
soil	$mg.kg_{dwt}^{-1}$	20 [c]	0.20	n.a.	3.0×10^{2}
groundwater	$\mu g.L^{-1}$	6.2	6.2×10^{-2}	n.a.	1.1×10^{2}
air	$\mu g.m^{-3}$	n.a.			

[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] The MPC_{soil} is based on the $MPC_{eco, soil}$ because human exposure through food consumption is considered not realistic.
n.a. = not applicable.

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