

RIVM report 601506005

BIOCIDES (II)

Refined aquatic environmental risk assessment
of 28 priority biocides

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Preface

This report is the follow-up of an inventory of biocides with serious data gaps (Mensink, 1999). For a substantial part of this group sufficient data could be obtained to perform a preliminary aquatic risk assessment: nevertheless, this first-tier approach includes various worst-case assumptions, when particular model input data were not known. The main purpose of this follow-up is to include more realistic scenarios by performing refined aquatic risk assessments, when possible. However, it remains tedious to judge the extent of realism of these scenarios as the actual conditions of various Dutch facilities have not been mapped: *e.g.* the waste water production of paper factories, whereas they are the starting-point of the aquatic risk assessment. Also, not many data are known on the role of sewage treatment plants, whereas their role is crucial for most of the biocides in this report. Therefore it is clear that the approach in itself is not sufficient to really characterise the actual hazards due to the use of these biocides, also due to the mere reason that there are almost no measurements of concentrations in process water or effluent. On the other hand, this report integrates many environmentally important data and is therefore a starting-point for further discussions on the (re)registration of these biocides. Also, I hope that this report is a help for the selection of substances and their applications that need further investigation or monitoring.

The exposure assessment is probably a much larger source of variation than the effects analysis. By pointing at the more well and the more ill-founded aspects of the refined risk assessment, I have tried to deal with these elements of variation. Also I have tried to capture the variation in outcomes by including as many scenarios as possible within the available time and this was the practical reason that *e.g.* for slimicides more scenarios have been included than for liquid-cooling system preservatives. Of course, the more scenarios can be used for a particular application, the more accurate the range of concentrations can be judged to which aquatic wildlife can be actually exposed.

As for its predecessor I hope that this report may facilitate the process of gaining relevant data for environmental risk assessment in an efficient way. Then we can hopefully draw conclusions on the environmental impact of this "lost" group of pesticides, satisfactorily for both the regulating authorities and the industries.

I would like to thank drs. Mark Montforts (RIVM/CSR) for critically reviewing this report.

In conclusion, I would like to quote — for the Dutch readers — Arthur Schopenhauer, the German philosopher:

..En toch is niets gemakkelijker dan zo te schrijven dat geen mens het begrijpt, zoals er ook niets moeilijkers is dan nuttige gedachten zo uit te drukken, dat iedereen ze wel móet begrijpen.

From: *Parerga und Paralipomena* (1851)

Abstract

This study assesses the risk for the aquatic environment posed by a "rest" group of 93 non-agricultural pesticides: so defined because they do not fit into any policy spearheads of the Dutch government on biocides. This "rest" group therefore represents a wide array of biocides with different structures and functions, varying from rodenticides and slimicides to liquid-cooling system preservatives and sanitary disinfectants. In a previous study 28 active ingredients and their applications — combined into a group of about 50 substance-specific applications (SSAs) — were considered potentially hazardous to the aquatic environment. This group represents the starting-point for the present study to answer the question: *what can be concluded about its harmfulness when more realistic scenarios are introduced?* This refined aquatic risk assessment revealed that a total of 26 SSAs are still considered to be potentially (very) hazardous. As the scenarios are assumed to contain more realistic elements, this particular group is more likely actually to have a negative impact on the aquatic wildlife. The actual extent of this impact, however, remains speculative. The group contains mainly of slimicides, liquid-cooling system preservatives and sanitary disinfectants. This group should be considered for further investigation in the approach of a tiered risk assessment. Then *e.g.* actual measurements in process water may be decisive for final conclusions. For this group of biocides policymaking might focus on: 1) availability of (refined) scenarios, 2) usefulness of (refined) scenarios and 3) validation of scenario calculations with monitoring data of process water and effluent. Outside this group of 26 SSAs, there are a few focal points as well; *e.g.* an important bottleneck is the absence of models for biocides in the food and feed fields, despite the probability that large numbers could be used here.

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Abbreviations & definitions

a.i.	active ingredient
BCF	bioconcentration factor: the ratio of the test substance concentration in fish to the concentration in water at steady state
blow-down	the water that is released from a recirculating cooling-water system to the recipient surface water to replace evaporated water in a cooling tower; this release can be directly or indirectly (via an STP) to surface water
CTB	Dutch Board for the Authorisation of Pesticides (In Dutch: College voor de Toelating van Bestrijdingsmiddelen)
CUWVO/CIW	Coördinatiecommissie Uitvoering Wet Verontreiniging Oppervlaktewateren/Commissie Integraal Waterbeheer
DT ₅₀	time in which 50% of the parent compound has disappeared from water, soil, or sediment by transformation
EC ₅₀	median effective concentration: 1. the concentration resulting in a 50% change in a parameter (<i>e.g.</i> algal growth) relative to the control 2. the concentration at which a particular effect (<i>e.g.</i> Daphnia immobilisation) is observed in 50% of the organism population relative to the control
EPIWIN	a QSPR* database
EU	European Union
EUSES	the European Union System for the Evaluation of Substances: an integrated risk assessment system
FAMRISK	acronym of those biocides for which preliminary risk assessment is possible: models are available and sufficient environmental data are available to run these models
K _{oc}	sorption coefficient corrected for the organic carbon content
K _p	sorption coefficient (<i>e.g.</i> for suspended matter or sediment)
LC ₅₀	median lethal concentration: a statistically derived concentration that can be expected to cause death in 50% of the exposed organisms for a specified time
max.	maximally

MATC	maximum acceptable toxicant concentration
MPA	maximum permissible addition (MPA is the MPC* minus the background concentration)
MPC	maximum permissible concentration (MPC is the MPA* plus the background concentration)
NOEC	no-observed-effect-concentration: the highest concentration without adverse effects
PEC	predicted environmental concentration: the expected concentration in an environmental compartment, calculated using a model
PNEC	predicted no-effect concentration
QSPR	a quantitative structure-property relationship
RCR	risk characterisation quotient
SSA	substance-specific application
SST	stofspezifieke toepassing
STP	sewage treatment plant
syn	synonym
UNFAMRISK	acronym of those biocides for which preliminary risk assessment is not possible: models are not available or insufficient environmental data are available to run these models
USES	Uniform System for the Evaluation of Substances: an integrated risk assessment system
VNCI	Vereniging van de Nederlandse Chemische Industrie

Samenvatting

De restgroepbiociden zijn een vergaarbak met 93 niet-landbouwbestrijdingsmiddelen, die indertijd niet in een van de vijf beleidsspeerpunten zijn geplaatst. In een eerdere studie werd voor 11 stoffen een potentieel risico voor waterorganismen vastgesteld. Bij nog eens 17 stoffen kon dit wegens gebrek aan voldoende gegevens niet worden vastgesteld, hoewel emissies niet konden worden uitgesloten. Deze actieve stoffen en hun toepassing zijn gekoppeld tot ca. 50 zogenaamde stofspecifieke toepassingen (SST's). Op deze ca. 50 SST's concentreert zich deze follow-up studie. Hierin is getracht om vast te stellen of onder realistischer omstandigheden nog steeds sprake zou zijn van potentiële risico's. Hierbij zijn de volgende productgroepen aan bod gekomen: antisljmstoffen in de papier- en suikerverwerkende industrie, sanitaire desinfectantia ten bate van de volksgezondheid, desinfectantia in de voedings- en veevoederindustrie, en die houtconserveringsmiddelen en koelwaterpreservatieven die niet in de speerpunten meegenomen zijn.

Na deze verfijnde risicobeoordeling bleken van de ca. 50 SST's er nog altijd 26 te zijn die worden verondersteld (zeer) schadelijk voor waterorganismen te zijn. Het gaat vooral om antisljmstoffen, koelwaterpreservatieven en sanitaire desinfectantia die tot deze "probleem"groep horen. Tevens bleken er 8 SST's niet schadelijk voor waterorganismen te zijn (houtverduurzamingsmiddelen en sanitaire desinfectantia). Van 16 SST's kon een dergelijke schadelijkheid nog altijd niet worden vastgesteld (vooral voor desinfectantia uit de voedingsindustrie). Cruciaal hierbij is hoe realistisch de scenario's zijn die voor de (zeer) milieuschadelijke SST's zijn doorgerekend. Slechts de resultaten van de koelwaterpreservatieven kunnen enigszins worden vergeleken met de resultaten van meer systematisch experimenteel onderzoek. Hierbij bleken de geschatte concentraties in het oppervlaktewater globaal over een te komen met de gemeten concentraties. Een knelpunt is het ontbreken van operationele risicomodellen voor biociden in de voedings- en veevoedersector.

Het beleid ten aanzien van de restgroepbiociden zal zich toe moeten spitsen op:

1. de beschikbaarheid en bruikbaarheid van scenario's: op grond van welke — meer of minder realistische — scenario's wil men beleidsbeslissingen nemen;
2. het vergelijken van monitoringsgegevens in proces- en afvalwater met berekende blootstellingsniveau's.

Deze punten zijn aan elkaar gerelateerd. Punt 1 lijkt meer een zaak van de evaluerende instanties (toelating van middelen) en punt 2 meer voor de waterkwaliteitsbeheerders. Het is van belang dat wat betreft de milieutechnische aspecten van "probleem"toepassingen in overleg zal worden getreden met de experts van de (emitterende) bedrijven zelf. Van de toepassingen waarvan nu nog steeds niet duidelijk

is in hoeverre er sprake is van schadelijkheid voor het aquatische milieu moet worden vastgesteld of deze leemtes moeten worden geslecht.

Summary

A "rest" group of 93 non-agricultural pesticides has been so defined because these pesticides do not fit into any of the five policy spearheads of the Dutch government on biocides. A potential risk of 11 substances for aquatic organisms was determined in a previous study. Hazard assessment was not possible for another 17 substances due to lack of environmental data, whereas emission to surface water — and therefore a potential risk — could not be excluded. These active ingredients and their applications were combined into about 50 substance-specific applications (SSAs). This follow-up investigation focuses on these approximately 50 SSAs, in an attempt to determine whether more realistic scenarios would still result in potential risks. The following product types were dealt with: slimicides in the paper and sugar industry, sanitary disinfectants in the public health area, disinfectants in the feed and food industry, and wood preservatives and cooling water preservatives that were not included in the spearheads.

After this refined aquatic risk assessment, 26 of the approximately 50 SSAs were and are still considered to be (very) hazardous to aquatic organisms. The biocides involved are mainly slimicides, cooling-water preservatives and sanitary disinfectants, making them "problematic" applications. Another 8 SSAs were found to be harmless (wood preservatives and sanitary disinfectants). It was still impossible to reach any conclusion for 16 SSAs (disinfectants in the feed and food field in particular; the lack of models in this field is a bottleneck), which render these applications "problematic" as well. A crucial factor here is the realism of the scenarios that identified the (very) hazardous SSAs: the actual extent of the negative impact on the aquatic wildlife remains speculative. For example, only for the cooling-water preservatives the results seem to be backed up by more systematic experimental evidence: *i.e.* estimated concentrations in the surface water match the measured concentrations.

For the "problematic" applications the policymaking might focus at:

1. availability and usefulness of scenarios: in view of which — more or less realistic — scenarios should policy decisions be taken?
2. validation of scenario calculations with monitoring data of process water and effluent.

Although these options are interrelated, the first might be dealt with by the registration authority (registration of products) and the second by the water quality authorities. It is important to involve the experts of the (emitting) industries in the discussion on the environmentally technical aspects of the "problematic" SSAs. Where scenarios are lacking, filling the gaps should be considered.

1. Introduction

A remaining group of 93 non-agricultural pesticides has been defined as such as they did not fit into any of the five policy spearheads of the Dutch government on biocides (Ameco, 1996; Mensink, 1999; de Heer, 2000). Therefore this “rest”group — the preferred designation in this present study — was a repository of a wide array of non-agricultural pesticides with very different structures and functions (see Fig. 1.1). A general feature, however, of this “rest”group was assumed to be that there was only a limited amount of environmental data. Nevertheless, for 22 substances and their applications it was shown in an RIVM study that there were enough data to perform a preliminary risk assessment for the aquatic environment (Mensink, 1999)¹: for these substances there were a minimum package of environmental data and an operational model for risk assessment, by which a PEC/PNEC ratio² could be calculated.

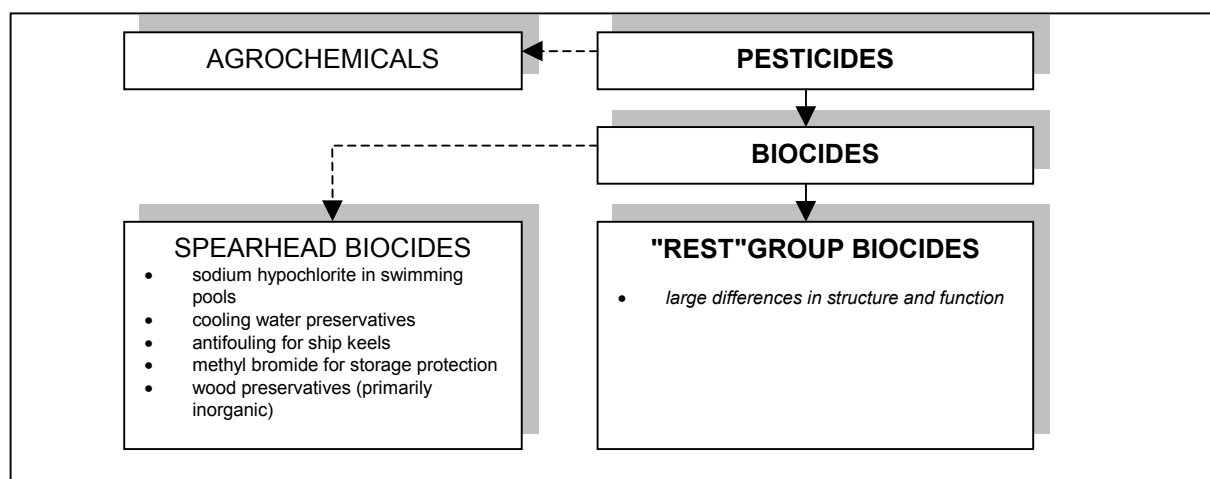


Fig. 1.1 The “rest”group biocides in relation to other pesticides.

It was assumed at the time that most biocides in the “rest”group probably did not affect the environment. However, by estimating the PEC/PNEC ratio, 11 substance-specific applications — e.g. 1,2-benzisothiazolin, when used as a slimicide in paper industries — could be characterised as potentially environmentally hazardous (Mensink, 1999). This equalled 50% of the substance-specific applications for which the PEC/PNEC

¹ Preliminary risk assessment implies a first-tier risk assessment based on a minimum amount of data and is generally referring to worst-case conditions. Therefore a preliminary (syn.: initial) risk assessment generally refers to potential rather than to actual risks. A refined risk assessment, however, generally refers to a more specified risk assessment that is more tuned to the actual conditions under which a biocide is used. When available, a more refined risk assessment is also based on more realistic environmental data, whereas preliminary assessments may be based on worst-case defaults.

² The PEC is the Predicted Environmental Concentration: the concentration in the surface water estimated by a model or based on actual measurements of a substance. The PNEC is the Predicted No-Effect Concentration: the highest concentration of a substance in the surface water that is assumed to cause no adverse effects to aquatic organisms. For most “rest”group biocides in the present study, the PNEC is extrapolated *c.q.* based on short-term toxicity tests with algae, crustaceans or fish.

ratio could be estimated and 28% of those for which toxicity-relevant emissions could not be excluded³.

The term *substance-specific application* has been chosen to emphasise that the extent of environmental hazardousness not only depends on the intrinsic properties of the substance itself but on the type of application of that substance as well. Therefore, in the context of this study, a particular substance is only discussed in combination with its application. For another 17 substance-specific applications, it was shown by Mensink (1999) that although PEC/PNEC ratios could not be estimated, local toxicity-relevant emissions could not be excluded in view of the available data. Therefore, the present study focuses on these two prioritised groups of 11 and 17 applications, as these groups are assumed to have the highest likelihood of impact on the aquatic ecosystem.

These two groups contained the substance-specific applications as listed in Tables 1.1 and 1.2. They have been given the acronyms FAMRISK — the risks are familiar, at least to some extent on a theoretical level — and UNFAMRISK, — the risks are unfamiliar — respectively. The applications of the FAMRISK biocides are potentially hazardous. The hazardousness of the applications of the UNFAMRISK biocides are not known, whereas toxicity-relevant emissions — *e.g.* via STPs — cannot be excluded. In

Table 1.1 The FAMRISK group: **preliminary risk assessment was possible** as models were available and at the same time sufficient environmental data were available to run these models (*e.g.* an LC_{50} of one of the three conventional trophic levels was considered sufficient to run USES or EUSES). The PEC/PNEC ratios of FAMRISK were shown to exceed 1.

substance	product type(s)	CAS no.
1. 1,2-benzisothiazolin-3-one	slimicide	2634-33-5
2. 2-phenyl-phenol	textile preservative	90-43-7
3. 2-(thio cyano methyl thio)benzothiazole	textile preservative	21564-17-0
4. 2,2-dibromo-3-nitropropionamide	slimicide; liquid-cooling preservative	10222-01-2
5. 2-bromo-4-hydroxyacetofenone	slimicide	2491-38-5
6. 2-methyl-4-isothiazolin-3-one	slimicide; liquid-cooling preservative; wood preservative <i>ic</i> by impregnation	2682-20-4
7. bromonitrostyrene	slimicide; liquid-cooling preservative	7166-19-0
8. dichlofluamide	in-can preservative; wood preservative <i>ic</i> by impregnation; antifouling	1085-98-9
9. formaldehyde	private area and public health disinfectant	50-00-0
10. sulcofuron	textile preservative	3567-25-7
11. zinc oxide	antifouling	1314-13-2

the acronyms (UN)FAMRISK the term RISK has been used for reasons of convenience. In the context of the present study it has no probabilistic meaning.

Rearranging the substance-specific applications in Tables 1.1 and 1.2 emphasising the product type gives Table 1.3. Three biocides — 2-phenyl-phenol, 2-(thio cyano methyl

³ Toxicity-relevant emissions are those of which adverse effects to aquatic organisms reasonably cannot be excluded. It is — of course — a qualitative term, but it reflects the notion that the occurrence of adverse effects *in situ* would not have surprised an expert completely. By using the term toxicity-relevant, a distinction is made between such emissions and other smaller emissions that are reasonably not expected to cause adverse effects anyway.

Table 1.2 The UNFAMRISK group: **preliminary risk assessment was not possible** as models or sufficient data to run these models were lacking. However, reasonably toxicity-relevant emissions could not be excluded.

substance	product type(s)	CAS no.
12. 2,2-dithio-bis-benzamide	in-can preservative; slimicide	2527-57-3
13. 4-chloro-3-methyl-phenolate sodium	in-can preservative	15733-22-9
14. 5-chloro-2-methyl-4-isothiazolin-3-one	slimicide; liquid-cooling preservative; industrial wood preservative	26172-55-4
15. 5-oxo-3,4-dichloro-1,2-dithiol	slimicide	1192-52-5
16. arsenic pentoxide	industrial wood preservative	1303-28-2
17. bromoacetic acid	preservative for beer breweries	79-08-3
18. cupric carbonate hydroxide	industrial wood preservative	12069-69-1
19. disodium cyanodithioimido carbonate	slimicide	138-93-2
20. glutaric aldehyde	slimicide; liquid-cooling preservative; preservative in the food and feed industry and private area and public health disinfectant	111-30-8
21. potassium bifluoride	wood preservative	7789-29-9
22. potassium hydroxide	private area and public health disinfectant; preservative in the food and feed industry; milking machine disinfectant	1310-58-3
23. potassium N-methyldithiocarbamate	slimicide	137-41-7
24. sodium dichloroisocyanurate	private area and public health disinfectant; preservative in the food and feed industry; milking machine disinfectant	2893-78-9
25. sodium hypochlorite	private area and public health disinfectant; liquid-cooling preservative; preservative in the food and feed industry; milking machine disinfectant	7681-52-9
26. sodium p-toluenesulfonchloramide	private area and public health disinfectant; preservative in the food and feed industry	127-65-1
27. zinc borate	private area and public health disinfectant; antifouling	1332-07-6
28. zinc oxalate	private area and public health disinfectant; antifouling	547-68-2

thio) benzothiazole and bromonitrostyrene — are not included in Table 1.3, as they already have been withdrawn from the market in 1999 and the last day for selling stored products has been expired.

In recapitulation, the following questions have been phrased:

1. Is it possible to refine the scenarios *c.q.* assumptions for the potentially hazardous applications of the FAMRISK group in such a way that there is more emphasis on realistic-case than on worst-case?

In this way the main purpose is to investigate whether PEC/PNEC ratios can be lowered, assuming that preliminary risk assessment reflects worst-case scenarios. Therefore this attempt to refined risk assessment is a top-down approach: once the PEC/PNEC ratio is ≤ 1 , further refinement is not necessary for that particular application, since then that particular substance-specific application is not expected to be environmentally hazardous anymore.

2. Is it possible to find or use data and models so that — at least— preliminary risk assessment for the aquatic organisms can be performed for the UNFAMRISK group?
3. Which substances and product types can be prioritised in view of the potentially hazardous applications, after refined risk assessment?

Table 1.3. *The abundance of the product types over FAMRISK and UNFAMRISK (product types in conformity with the EU designations, see Appendix 3)*

product type	FAMRISK	UNFAMRISK	TOTAL
SLIMICIDE	4	6	10
PRIVATE AREA/PUBLIC HEALTH DISINFECTANS	1	7	8
PRESERVATIVE FOOD/FEED INDUSTRY		6	6
WOOD PRESERVATIVE	2	4	6
COOLING SYSTEM PRESERVATIVE	2	3	5
ANTIFOULING*	2	2	4
MILKING MACHINE DISINFECTANS		3	3
IN-CAN PRESERVATIVE	1	2	3
TEXTILE PRESERVATIVE	1		1
TOTAL	13	33	46

* zinc oxide, zinc oxalate and zink borate were ingredients of the product ALBOFIX. All these ingredients were classified as antifouling in view of the legal regulation and usage instructions⁴. As these instructions were not always clear whether it could be used for ship keels, this classification may be debatable.

The present study has been performed by order of and in close co-operation with the Directorate-General for Environmental Protection. The findings of the DGEP are reported in De Heer (2000).

The following bookmark provides some useful hints for the reader:

- **Chapter 1** Introduction, context, and scientific questions for the investigation;
- **Chapter 2** Methodology: the tools that are used for hazard classification and risk assessment;
- **Chapter 3** Results: which substances and their applications are questionable for the aquatic environment; which data are still lacking;
- **Chapter 4** Conclusions and discussion: what is the relevance of the present study, what can be done with the results, what are the possibilities for further assessment refining;

- **Appendix 1** *Refined risk assessment for the aquatic environment per priority substance: the available data on physico-chemical properties, environmental and ecotoxicological endpoints, the PEC/PNEC ratios and the corresponding hazard groups per product type, and a discussion on the relevant aspects of the refined risk assessment that are involved;*

- **Appendix 2** *The EU biocidal product types: a short subscription;*

- **Appendix 3** *Risk characterisation (PEC/PNEC ratios) spreadsheets per priority substance: listing the PNEC and its source for derivation, the PECs per application, the number of scenarios per substance showing a (very) hazardous application and some of the relevant assumptions for running the models;*

- **Appendix 4** *Mailing list.*

⁴ Wettelijk gebruiksvoorschrift en gebruiksaanwijzing (in Dutch).

2. Methodology

Firstly, a subdivision has been made within the prioritised chemicals. Based on the abundance of product types as listed in Table 1.3, only those product types have been selected that were represented by at least 5 applications. Therefore the following product types have been taken into account (in decreasing order): slimicides (10 substance-specific applications), private area and public health area disinfectants and other biocidal products (8), food and feed area disinfectants (6), wood preservatives (6) and preservatives for liquid-cooling and processing systems (5). In this way c. 50 of the 193 substance-specific applications — the original number that was gathered on the “rest” group list with the 93 biocides — have been taken into account in the present study. Hereby, it should be noted that the same particular active ingredient may be used in different product types and therefore in more substance-specific applications.

Secondly, the following substance-specific applications have been defined with respect to the PEC/PNEC ratio for aquatic organisms in the recipient surface water (see Fig. 2.1; for further explanation, see text below).

The integrated risk assessment model (E)USES (EC-EUSES, 1996; RIVM, VROM & VWS, 1998) is used for estimating PEC values in the recipient water. PNECs are derived in conformity with Kalf *et al.* (1999).

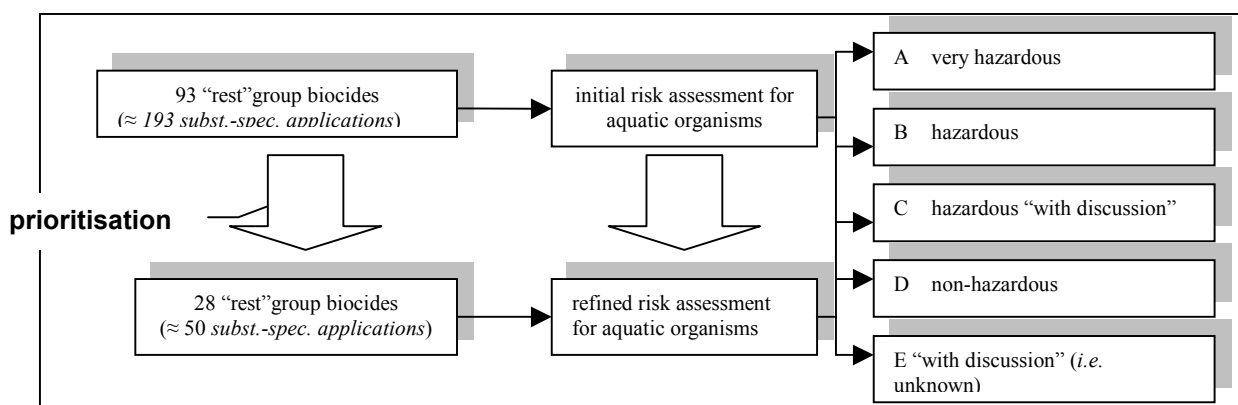


Fig. 2.1 The process of prioritisation, risk assessment and hazard classification in this study (subst.-spec. is substance-specific).

The results of the refined risk assessment allow a hazard classification, as represented in Fig. 2.1 (this classification should be seen in the context of the present study only):

- A. **very hazardous applications:** those that indicate hazards to the aquatic environment with a $\frac{PEC}{PNEC} > 100$ for at least one of the refined risk assessment scenarios in this report.
- B. **hazardous applications:** those that indicate hazards to the aquatic environment with $10 < \frac{PEC}{PNEC} \leq 100$ for at least one of the refined risk assessment scenarios in this report.

- C. **hazardous applications “with discussion”**: those that indicate hazards to the aquatic environment with $1 < \frac{PEC}{PNEC} \leq 10$ for at least one of the refined risk assessment scenarios in this report. It is assumed that a relatively small adjustment of the underlying assumptions may result into an opposite conclusion (*i.e.* non-hazardous instead of hazardous). Therefore the alleged hazardousness of these applications is assumed to be more disputable than for A and B. A more detailed discussion on the assumptions may be more relevant than for the other (very) hazardous applications A and B.
- D. **non-hazardous application**: those that show $\frac{PEC}{PNEC} \leq 1$ for all the registered applications. Apparently, there is no scenario available in which the PEC exceed the PNEC. It is assumed not necessary to investigate whether some less realistic assumptions need to be adjusted, as the PEC is already below the effect level.
- E. **application “with discussion”**: those for which a refined environmental risk assessment is (still) not possible: crucial data may be lacking or a proper model may not be available. Therefore discussion about these biocides remains necessary.

The first three groups — very hazardous, hazardous, and hazardous “with discussion” — indicate that there may be a risk: a non-negligible probability that a PEC exceeds a PNEC. However, it does not indicate this probability itself, and therefore it does not indicate that a “very hazardous” substance-specific application has a stronger environmental impact than a “hazardous” or a “hazardous with discussion” application. Only the group of non-hazardous substances indicate that there is no risk: the probability that a PEC exceeds a PNEC is assumed to be nil. Only for category E — an application “with discussion” — a PEC/PNEC ratio cannot be determined, indicating that the discussion with respect to this substance-specific application should be continued.

3. Results

The most important results are summarised in Table 3.1. Some of the substance-specific applications have recently been withdrawn from the Dutch market. This was generally not due to their environmental impact. Too high costs for submitting test data required by the CTB or other commercial reasons appear to be more important reasons for withdrawal. It is important to note this as it may imply that biocides that are now withdrawn from the market — and therefore skipped for risk analysis — may be remarketed in the near future. An example is BUSAN 30L with the active ingredient 2-(thio cyano methyl thio) benzothiazole as a wood preservative. At the reference date for the present study no products with 2-(thio cyano methyl thio) benzothiazole were on the Dutch market, suggesting that all products have been withdrawn (as this a.i. was on the original reference list of "rest" group biocides, see Ameco, 1996 and CREM, 1996). However, this wood preservative is in the process of registration since 1997 and as the CTB hasn't decided yet on its approval it may be remarketed in the near future. It should also be noted that some of these withdrawn biocides may still be sold until their stock is exhausted.

Withdrawn substance-specific applications in Table 3.1 are some textile preservatives (2-phenyl-phenol, 2-(thio cyano methyl thio)benzothiazole, and sulcofuron), slimicides (bromonitrostyrene and 5-oxo-3,4-dichloro-1,2-dithiol), private area and public health area disinfectants (zinc borate and zinc oxalate). Most of these withdrawals could not be taken along in the calculations as they were too recent.

It can be deduced from Table 3.1 that among the prioritised biocides there are:

- 26 "problematic" substance-specific applications (A,B, and C classifications)

Even after refined risk assessment these applications are still assumed to be (very) hazardous to the aquatic environment. This group contains primarily slimicides, liquid-cooling preservatives, and sanitary disinfectants. Sanitary disinfectants appear to have a broader range of PEC/PNEC ratios than the other product types. This group contains predominantly strongly reactive chlorine splitting off chemicals like sodium dichloroisocyanurate, sodium hypochlorite and sodium p-toluenesulfonchloramide. Within this group there are 5 applications for which the PEC exceeds the PNEC, but only to a limited extent (max. 10 times).

- 8 "non-problematic" substance-specific applications (D classification)

This group contains e.g. the use of glutaric aldehyde when disinfecting endoscopes in hospitals. It also contains some substances for wood preservation: potassium bifluoride (when used in plugs), cupric carbonate hydroxide and dichlofluanide.

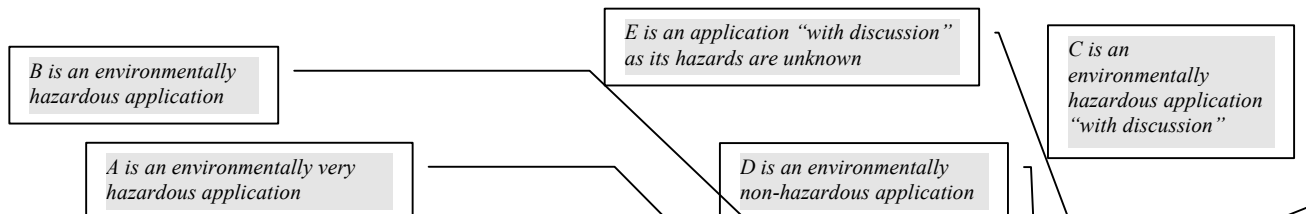


Table 3.1 The priority biocides and their (presumed) hazards.

		EU PRODUCT TYPE	HAZARD CLASSIFICATION					
			environmentally (very) hazardous application	A	B	C	D	E
	PRIORITY BIOCIDES							
1	1,2-benzisothiazolin-3-one	slimicide	▼					
2	2-phenyl-phenol	textile preservative	withdrawn from the market					
3	2-(thio cyano methyl thio)benzothiazole	textile preservative	withdrawn from the market					
4	2,2-dibromo-3-nitropropionamide	slimicide	▼					
		liquid-cooling preservative	▼					
5	2-bromo-4-hydroxyacetofenone	slimicide	▼					
6	2-methyl-4-isothiazolin-3-one	slimicide		▼				
		liquid-cooling preservative	▼					
		wood preservative <i>ic</i> by impregnation		▼				
7	bromonitrostyrene	slimicide	withdrawn from the market					
		liquid-cooling preservative	withdrawn from the market					
8	dichlofluanide	in-can preservative					▼	
		wood preservative <i>ic</i> by impregnation				▼		
		antifouling					▼	
9	formaldehyde	public health area (medical equipment)			▼			
		public health area (accommodations man)				▼		
		public health area (chemical toilets)					▼	
		public health area (other)			▼			
10	sulcofuron	textile preservative	withdrawn from the market					
11	zinc oxide	antifouling					▼	
12	2,2-dithio-bis-benzamide	in-can preservative					▼	
		slimicide					▼	
13	4-chloro-3-methyl-phenolate sodium	in-can preservative					▼	
14	5-chloro-2-methyl-4-isothiazolin-3-one	slimicide		▼				
		liquid-cooling preservative	▼					
		wood preservative <i>ic</i> by impregnation		▼				
15	5-oxo-3,4-dichloro-1,2-dithiol	slimicide	▼	withdrawn from the market				
16	arsenic pentoxide	industrial wood preservative				▼ ⁵	▼ ⁶	
17	bromoacetic acid	food & feed area					▼	
18	cupric carbonate hydroxide	wood preservative <i>ic</i> by impregnation				▼ ⁷	▼ ⁸	
19	disodium cyanodithioimido carbonate	slimicide	▼					
20	glutaric aldehyde	slimicide	▼					
		liquid-cooling preservative	▼					
		food & feed area					▼	
		public health area (medical equipment)			▼			
		public health area (accommodations man)				▼		
	public health area (other)				▼			
21	potassium bifluoride	wood preservative				▼		
22	potassium hydroxide	public health area (medical equipment)				▼		
		food & feed area					▼	

⁵ refers to emissions during impregnation.

⁶ refers to direct leaching from sheet piles into the surface water.

⁷ see footnote 5.

⁸ see footnote 6.

Table 3.1 (Contd.)

	EU PRODUCT TYPE	HAZARD CLASSIFICATION				
		A	B	C	D	E
23	potassium N-methyldithiocarbamate slimicide	▼				
		environmentally (very) hazardous application				
	PRIORITY BIOCIDES					
24	sodium dichloroisocyanurate	public health area (swimming pool)	▼			
		public health area (accommodations man)	▼			
		public health area (other)	▼			
		food & feed area				▼
25	sodium hypochlorite	public health area (accommodations man)	▼			
		public health area (other)		▼		
		food & feed area				▼
		liquid-cooling preservative	▼			
26	sodium p-toluenesulfonchloramide	public health area (accommodations man)			▼	
		public health area (other)			▼	
		food & feed area				▼
27	zinc borate	public health area (accommodations man)	withdrawn from the market			
		antifouling	withdrawn from the market			
28	zinc oxalate	public health area (accommodations man)	withdrawn from the market			
		antifouling	withdrawn from the market			
TOTAL NUMBER OF SUBSTANCE-SPECIFIC APPLICATIONS		16	5	5	8	16

B is an environmentally hazardous application
A is an environmentally very hazardous application
E is an application "with discussion" as its hazards are unknown
D is an environmentally non-hazardous application
C is an environmentally hazardous application "with discussion"

- 16 substance-specific applications without sufficient data or models for initial or refined risk assessment (E classification)

Additional data are currently required by the CTB for most chemicals in this group, but not for all members of this group like disodium cyanodithioimido carbonate and potassium N-methyldithiocarbamate, two pesticides that are both used in one product in sugar processing industries. An important bottleneck is the lack of operational risk assessment models in the food and feed industries. Substances of this product type can be used in huge quantities, e.g. sodium dichloroisocyanurate, bromoacetic acid and potassium hydroxide. The latter — in 1992 probably the biocide with the second highest usage rate in the Netherlands with 335,000 tons — is rather a eutrophication agent than an ecotoxicant.

The expiration dates for the 26 "problematic" applications are listed in Table 3.2.

Table 3.2 Expiration data for the 26 "problematic" substance-specific applications. The number of registrants is included for a limited number of biocides (reference date 05-03-2000): only those with a PEC/PNEC ratio >1 in view of the initial risk assessment (see Mensink, 1999) (grey in the Table)

	PRIORITISED BIOCIDES	EU PRODUCT TYPE	NUMBER OF REGISTRANTS OF A PARTICULAR APPLICATION	DATE OF EXPIRATION OR FOR SELLING THE LAST STOCKS
1	1,2-benzisothiazolin-3-one	slimicide	1	01-01-2001
4	2,2-dibromo-3-nitropropionamide	slimicide	9	01-06-2001
		liquid-cooling preservative		01-06-2001
5	2-bromo-4-hydroxyacetofenone	slimicide	1	01-02-2002
6	2-methyl-4-isothiazolin-3-one	slimicide	13	01-01-2002
		liquid-cooling preservative		01-01-2002
		wood preservative (impregnate)		01-01-2002
9	formaldehyde	san. disinfectant (med. equip.)	≤22	01-10-2000
		san. disinfectant (other)		
14	5-chloro-2-methyl-4-isothiazolin-3-one	slimicide		01-01-2002
		liquid-cooling preservative		01-01-2002
		wood preservative (impregnate)		01-01-2002
15	5-oxo-3,4-dichloro-1,2-dithiol	slimicide		last selling date : 01-07-2000
19	disodium cyanodithioimido carbonate	slimicide		01-11-2001
20	glutaric aldehyde	liquid-cooling preservative		01-10-2000
		san. disinfectant (med. equip.)		
23	potassium N-methyldithiocarbamate	slimicide		01-11-2001
24	sodium dichloroisocyanurate	san. disinfectant (swimming pool)		01-11-2000
		san. disinfectant (housekeeping, hospital)		01-11-2000
		san. disinfectant (other)		01-11-2000
25	sodium hypochlorite	san. disinfectant (housekeeping, hospital)		01-10-2001
		san. disinfectant (other)		
26	sodium p-toluenesulfonylchloramide	san. disinfectant (housekeeping, hospital)		01-09-2001
		san. disinfectant (other)		

4. Conclusions and discussion

The following applications are still assumed to be (very) hazardous to the aquatic environment: liquid-cooling preservatives, slimicides, and sanitary disinfectants. An important bottleneck is the lack of operational risk assessment models in the food and feed industries.

When considering the results of the refined risk assessment for aquatic organisms, it is, of course, crucial to have a proper understanding how realistic the chosen scenarios are that underlie the model calculations.

Firstly, it is important to note that for most of the "problematic" applications — *i.e.* the 26 applications with a PEC exceeding the PNEC — there are also scenarios for the same application that indicate no hazards (see *e.g.* Appendix 3, p. 87 on 2,2-dibromo-3-nitrilopropionamide). Thus it is important to find the reasons for these differences. However, that was beyond the scope of the present study. There is one product type that is an obvious exception to this rule: the liquid-cooling preservatives. Refined risk assessment for this product type gives much larger PEC/PNEC ratios than the initial risk assessments. However, for these preservatives only 1-3 scenarios have been calculated whereas for other product types the number of scenarios may increase up to 12 scenarios per substance-specific application. Therefore the inclusion of more scenarios for the liquid-cooling preservatives may reveal more non-hazardous applications as well. On the other hand, liquid-cooling preservatives are among the few product types of biocides that have been subjected to a more thorough empirical investigation in the Netherlands (see *e.g.* Baltus & Berbee, 1996, and Baltus *et al.* 1999) and the results of these investigations link up with those in the present study.

The exposure assessment appears to be the most vulnerable part of the PEC/PNEC approach. The behaviour of biocides in the plants or facilities where they are used is often more complicated than the model outcomes suggest, and therefore this is often the reason why the confidence limits around this average PEC are assumed to be large. Of course this is a fierce limitation when interpreting the results. On the other hand: these ratios may give a clue for further research as monitoring data — which definitely could substitute the PECs generated by the models in this report — are often not available or in a small number at most. Therefore the PEC/PNEC approach should be seen as the most feasible approach, until better data — particularly the actual concentrations under domestic or industrial conditions — become available.

Secondly, an important limitation in the use of the PEC/PNEC ratio approach, is that it does not inform on the probability that the exceeding of the PNEC is expected to happen: twice a year or — let's say — once per twenty years. However, though the

PEC/PNEC concept may be less helpful in truly identifying the actual environmental risks it has been acknowledged as a decisive cutoff value in the decision-tree for granting (re)registration (ECB, 1996).

In conclusion, the question to what extent the results of the present study are relevant for policymaking remains uneasy to answer. The outcomes of this study do not give an indication how frequent no-effect levels are exceeded and it is not clear to what extent the assumptions in the respective scenarios really reflect the circumstances in the Netherlands. Therefore the final discussion aggravates on two issues:

1. to what extent do the models — used in this study — correspond with the typical or atypical circumstances in the Netherlands? Are for example the Finnish paper mill scenarios that have been used in this study comparable with a typical scenario of a Dutch paper mill? Besides, under particular conditions the dilution factor of the purified effluent to the recipient water is 1 (Seppälä, 2000), whereas in the Netherlands often a dilution factor of 10 is taken into account. For several product types new scenarios need to be developed (*e.g.* in the food and feed area).
2. do reliable chemical analyses of process or waste water confirm or contradict the picture that has been outlined by the PEC/PNEC ratio approach in this study? The few actual analytical measurements that have been collected in the context of this study fit within the model-estimated ranges.

The issues 1 and 2 are, of course, interrelated. Issue 1, however, can be dealt with by the pesticide evaluating authorities, whereas issue 2 may be broached by the national and regional water quality authorities or the CUWVO/CIW. Only recently, it has been drawn up by law that a number of CTB approved biocides may only be used after authorisation of the local water quality authorities: *e.g.* AQUACID 39D, a slimicide in the paper and cardboard industries with the active ingredients 2-methyl-4-isothiazolin-3-one and 5-chloro-2-methyl-4-isothiazolin-3-one.

In summary, it can be stated that it is possible to refine the scenarios of the preliminary risk assessment. Their scale of realism, however, is disputable, mainly because environmental data may still be lacking, and typical conditions of Dutch facilities may not resemble those of the used scenarios (*e.g.* a Finnish model for slimicides). A top-down approach to see whether RCRs can be lowered seems useful in this respect. Prioritised biocides after refined risk assessment are mainly slimicides, liquid-cooling system preservatives, and sanitary disinfectants.

It is, beyond any doubt, of crucial importance that with respect to the environmental-technical aspects of “problematic” applications — as defined in this study — an open and fruitful information exchange between the industries and the evaluating authorities is essential. Companies and industries may be challenged to judge the scenarios in the present study: to what extent do they reflect the conditions in their facilities? Only then it will be possible to pinpoint the factual problems, prior to solving them.

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Appendix 1

Refined risk assessment per priority substance

1

CAS no. 2634-33-5

1,2-benzisothiazolin-3-one

Syn.: 1,2-benzisothiazol-3(2H)-one

molecular weight	vapour pressure	water solubility	log K _{ow}
(-)	(Pa)	(mg/litre)	(-)
151.2	5.8×10 ⁻⁵ *	500*	1.3

* at 20° C.

AQUATIC ENVIRONMENTAL/ECOTOXICOLOGICAL ENDPOINTS							
DT ₅₀ (hydrolysis)	DT ₅₀ (photolysis in water)	DT ₅₀ (biodegradation in water)	EC ₅₀ (STP microbes)	EC ₅₀ (algae)	E(L)C ₅₀ (crustaceans)	LC ₅₀ (fish)	BCF (fish)
(days)	(days)	(days)	(mg/litre)	(mg/litre)	(mg/litre)	(mg/litre)	(-)
11	-	1*	>>2	-	1.1**	1.2-4.8**	5.8-8.9

* EPIWIN indicates a probability of rapid biodegradation of 0.7.

** refers to the a.i. of a 78% product.

PRODUCT TYPE & EMISSIONS						
PRODUCT TYPE	SHORT DESCRIPTION	EMISSIONS EXPECTED TO*,**				
(code)		STP	SURFACE WATER	SEDIMENT	SOIL	OUTDOOR AIR
12.1	Slimicide, paper industry	EQ ¹	EQ ²	EQ ³	EQ ⁴	N ⁵

* for notes: see table on preliminary environmental risk assessment in Mensink (1999).

** Y = yes; N = no; EQ = equivocal.

RCRs INITIAL & REFINED RISK ASSESSMENT & HAZARD GROUP					
PRODUCT TYPE	SHORT DESCRIPTION	RCR*			HAZARD GROUP
(code)		INITIAL	LOWEST	HIGHEST	
12.1	Slimicide, paper industry	3627	1.8	2600	VERY HAZARDOUS APPLICATION

* for further details see Appendix 3, p. 89.

REFINED ENVIRONMENTAL RISK ASSESSMENT

There are conflicting data on the actual use rate of 1,2-benzisothiazolin-3-one in the Netherlands. Therefore, the emission patterns are unclear, and so, substantial emissions to STPs and, possibly, to surface waters and their corresponding sediments cannot be excluded, particularly when used in paper industries. However, refined risk assessment shows that 1,2-benzisothiazolin-3-one is a very hazardous substance, when used as slimicide, if USES 2.0 is used: it shows an RCR of 2600 (initial risk assessment: RCR is 3627). A Finnish model — that may be more realistic as it includes process temperature dependent hydrolysis and degradation — shows much lower RCRs of 0.18-0.27, when introducing an additional dilution factor of 10. This appears to indicate that hazards may turn out better than expected. However, there are no monitoring data to verify the exposure analysis.

CTB stated on 11-06-1999 that for a product with 1,2-benzisothiazolin-3-one PROXEL GXL — to be used in water-based products or as a slimicide — additional environmental data should be submitted by the registrant as prerequisites for reregistration: with respect to 1,2-benzisothiazolin-3-one these data should include chronic toxicity to crustaceans, chronic toxicity to fish (28-days juvenile growth test) and chronic toxicity to the sediment dwelling larvae of *Chironomus*.

2

CAS no. 90-43-7

2-phenyl-phenol

Syn.: o-phenyl-phenol; biphenyl-2-ol; (1-1'-biphenyl)-2-ol

molecular weight	vapour pressure	water solubility	log K _{ow}
(-)	(Pa)	(mg/litre)	(-)
170.2	0.07*	700**	3.2-3.4

* at 20 °C.

** at 25 °C.

AQUATIC ENVIRONMENTAL/ECOTOXICOLOGICAL ENDPOINTS							
DT ₅₀ (hydrolysis)	DT ₅₀ (photolysis in water)	DT ₅₀ (biodegradation in water)	EC ₅₀ (STP microbes)	EC ₅₀ (algae)	E(L)C ₅₀ (crustaceans)	LC ₅₀ (fish)	BCF (fish)
(days)	(days)	(days)	(mg/litre)	(mg/litre)	(mg/litre)	(mg/litre)	(-)
-	-	4-8*	-	43**	1.5	6-41	150

* EPIWIN indicates a probability of rapid biodegradation of >0.9.

** NOEC (algae) is 18 mg/litre.

PRODUCT TYPE & EMISSIONS						
PRODUCT TYPE	SHORT DESCRIPTION	EMISSIONS EXPECTED TO*,**				
(code)		STP	SURFACE WATER	SEDI-MENT	SOIL	OUTDOOR AIR
9.1	Fibre/polymer preservative (textile)	Y ¹	EQ ²	EQ ³	EQ ⁴	N ⁵

* for notes: see table on preliminary environmental risk assessment in Mensink (1999).

** Y = yes; N = no; EQ = equivocal.

REFINED ENVIRONMENTAL RISK ASSESSMENT
All registrations with 2-phenyl-phenol have been withdrawn from the market. Therefore no further refined risk assessment is needed.

3

CAS no. 21564-17-0

2-(thio cyano methyl thio)benzothiazole

Syn.: TCMTB

molecular weight	vapour pressure	water solubility	log K _{ow}
(-)	(Pa)	(mg/litre)	(-)
238.4	607*	20	3.1

* at 20 °C.

AQUATIC ENVIRONMENTAL/ECOTOXICOLOGICAL ENDPOINTS							
DT ₅₀ (hydrolysis)	DT ₅₀ (photolysis in water)	DT ₅₀ (biodegradation in water)	EC ₅₀ (STP microbes)	EC ₅₀ (algae)	E(L)C ₅₀ (crustaceans)	LC ₅₀ (fish)	BCF (fish)
(days)	(days)	(days)	(mg/litre)	(mg/litre)	(mg/litre)	(mg/litre)	(-)
68	< 1	2.8*	-	0.026**	0.022	0.021	184

* EPIWIN indicates a probability of rapid biodegradation of 0.4-0.6.

** refers to the a.i. of a 26% product. The NOEC (algae) of a 31% product was 0.0099 mg/litre (refers to a.i.).

PRODUCT TYPE & EMISSIONS						
PRODUCT TYPE	SHORT DESCRIPTION	EMISSIONS EXPECTED TO*,**				
(code)		STP	SURFACE WATER	SEDI-MENT	SOIL	OUTDOOR AIR
9.1	Fibre/polymer preservative (textile)	EQ ¹	EQ ²	EQ ³	EQ ⁴	N ⁵

* for notes: see table on preliminary environmental risk assessment in Mensink (1999).

** Y = yes; N = no; EQ = equivocal.

REFINED ENVIRONMENTAL RISK ASSESSMENT
All registrations with 2-(thio cyano methyl thio)benzothiazole have been withdrawn from the market. Therefore no further refined risk assessment is needed.

4

CAS no. 10222-01-2

2,2-dibromo-3-nitrilopropionamide

Syn.: DBNPA

molecular weight	vapour pressure	water solubility	log K _{ow}
(-)	(Pa)	(mg/litre)	(-)
241.8	0.0017*	1500	7.7**

* at 20 °C.

** EPIWIN estimate: 1.0. Estimate KEMI: 0,84 (Eriksson *et al.*, 1995)

AQUATIC ENVIRONMENTAL/ECOTOXICOLOGICAL ENDPOINTS							
DT ₅₀ (hydrolysis)	DT ₅₀ (photolysis in water)	DT ₅₀ (biodegradation in water)	EC ₅₀ (STP microbes)	EC ₅₀ (algae)	E(L)C ₅₀ (crustaceans)	LC ₅₀ (fish)	BCF (fish)
(days)	(days)	(days)	(mg/litre)	(mg/litre)	(mg/litre)	(mg/litre)	(-)
2.6	-	0.21	>2	0.3**	0.5-13	1-1.8***	13

*EPIWIN indicates a probability of rapid biodegradation of 0.02-0.9. KEMI estimate of 0.21 d (Eriksson *et al.*, 1995).

** NOEC (algae) is 0.02 mg/litre.

*** ELS tests show a 25-d NOEC of 0.47 mg/litre (hatching, embryo mortality) and a 60-85-d LC50 of 1.0-2.0 mg/litre (larval mortality).

PRODUCT TYPE & EMISSIONS						
PRODUCT TYPE	SHORT DESCRIPTION	EMISSIONS EXPECTED TO*,**				
(code)		STP	SURFACE WATER	SEDI-MENT	SOIL	OUTDOOR AIR
11 12.1	Liquid-cooling system preservative Slimicide (paper industry)	N ¹ EQ ¹	EQ ² EQ ²	EQ ³ EQ ³	EQ ⁴ EQ ⁴	N ⁵ N ⁵

* for notes: see table on preliminary environmental risk assessment in Mensink (1999).

** Y = yes; N = no; EQ = equivocal.

RCRs INITIAL & REFINED RISK ASSESSMENT & HAZARD GROUP					
PRODUCT TYPE	SHORT DESCRIPTION	RCR*			HAZARD GROUP
(code)		INITIAL	LOWEST	HIGHEST	
11	Liquid-cooling system preservative	400	2787	29000	VERY HAZARDOUS APPLICATION
12.1	Slimicide (paper industry)	833	0.01	573	VERY HAZARDOUS APPLICATION

* for further details see Appendix 3, p. 87 & 109.

REFINED ENVIRONMENTAL RISK ASSESSMENT

Refined risk assessment shows that 2,2-dibromo-3-nitrilopropionamide is a very hazardous substance. It hydrolyses very rapidly and therefore it seems plausible that (a) major metabolite(s) contribute(s) to the intrinsic toxicity to aquatic organisms. For at least one of the major metabolites this has been confirmed. Refined risk assessment shows that as a liquid-cooling system preservative the RCRs of the refined risk assessment are higher than those of the initial. This may imply that for water-cooling biocides the “default” assumptions of the initial risk assessment rather refer to typical than to atypical conditions. This appears to be confirmed by a few measurements of 2,2-dibromo-3-nitrilopropionamide in the blow-down of a Dutch electricity plant with an RCR of the parent compound of 40,000 (based on a measured concentration of 12,000 µg/litre; Baltus *et al.*, 1999). Addition of its probable major hydrolysis product — which was measured at a rate of 18,000 µg/litre — would even result in an RCR of 100,000 assuming that the PNEC is actually based on a mixture of the parent compound and its major hydrolytes (the parent compound hydrolysis readily, particularly at pH >8). It should be noted, however, that these RCRs refer to the undiluted blow-down before purification by biological treatment, so the actual RCRs in the recipient surface water can be expected to be lower (assuming a dilution factor of 10 only for the dilution — as default for USES 2.0 — would give RCRs of max. 10,000). Besides, this electricity plant was the only one — in a group of 14 facilities using cooling-water biocides — that used 2,2-dibromo-3-nitrilopropionamide. This plant used 200 kg/year, and 2,2-dibromo-3-nitrilopropionamide was applied intermittently for periods of 1.5 hours. The hazardousness of 2,2-dibromo-3-nitrilopropionamide as a cooling-water biocide for the aquatic environment was also reported by Baltus *et al.* (1999). They stated that in toxicity tests 2,2-dibromo-3-nitrilopropionamide containing effluent of 1 facility was acutely toxic to crustaceans and fish.

When used as a slimicide, the RCR range is much wider: only the USES scenarios indicate that the substance is very hazardous, whereas the Finnish and Swedish scenarios indicate that the substance can be non-hazardous as well, depending on the specific assumptions on hydrolysis and degradation in the plants prior to discharging the blow-down to the recipient water. However, the Finnish model — showing RCRs of 0.001-0.1, indicating no hazard with an additional dilution factor of 10 for the STP effluent to the recipient surface water — may be more realistic as it includes process temperature dependent hydrolysis and degradation. This indicates that hazards may turn out better than expected. However, there are no monitoring in the effluent of paper mills to verify the exposure analysis.

There is no specific legislative restriction that 2,2-dibromo-3-nitrilopropionamide is only allowed to be used if there are no direct or indirect emissions to surface water (as there is for *e.g.* 2-bromo-2-nitropropanediol 1-3, also one of the 93 “rest” group biocides, see Mensink, 1999).

5

CAS no. 2491-38-5

2-bromo-4-hydroxyacetofenone

molecular weight	vapour pressure	water solubility	log K _{ow}
(-)	(Pa)	(mg/litre)	(-)
214.9	6.8×10 ⁻⁴ *	1140	1.9**

* at 30 °C (EPIWIN estimate of the vapour pressure at 25 °C is 0.024 Pa).

** at pH 7.

AQUATIC ENVIRONMENTAL/ECOTOXICOLOGICAL ENDPOINTS							
DT ₅₀ (hydrolysis)	DT ₅₀ (photolysis in water)	DT ₅₀ (biodegradation in water)	EC ₅₀ (STP microbes)	EC ₅₀ (algae)	E(L)C ₅₀ (crustaceans)	LC ₅₀ (fish)	BCF (fish)
(days)	(days)	(days)	(mg/litre)	(mg/litre)	(mg/litre)	(mg/litre)	(-)
16	< 1	2.8*	-	-	1.8-3.2**	0.61-1.7***	-

* EPIWIN indicates a probability of rapid biodegradation of 0.02-0.7.

** refer to a.i of 27-47% products; 21-days NOEC (crustaceans) is 0.014 mg a.i./litre. The EPA (1995) derived an MATC for *Daphnia magna* of 0.09 mg a.i./litre.

*** refer to a.i of 27-47% products.

PRODUCT TYPE & EMISSIONS						
PRODUCT TYPE	SHORT DESCRIPTION	EMISSIONS EXPECTED TO*,**				
(code)		STP	SURFACE WATER	SEDI-MENT	SOIL	OUTDOOR AIR
12.1	Slimicide (paper industry)	EQ ¹	EQ ²	EQ ³	EQ ⁴	N ⁵

* for notes: see table on preliminary environmental risk assessment in Mensink (1999).

** Y = yes; N = no; EQ = equivocal.

RCRs INITIAL & REFINED RISK ASSESSMENT & HAZARD GROUP					
PRODUCT TYPE	SHORT DESCRIPTION	RCR*			HAZARD GROUP
(code)		INITIAL	LOWEST	HIGHEST	
12.1	Slimicide (paper industry)	28571	1	1289	VERY HAZARDOUS APPLICATION

* for further details see Appendix 3, p. 88.

REFINED ENVIRONMENTAL RISK ASSESSMENT

Refined risk assessment shows that 2-bromo-4-hydroxyacetofenone is a very hazardous substance. It hydrolyses moderately and is readily degradable in an STP. When used as a slimicide, the RCR range is very wide: all scenarios however, indicate that for 2-bromo-4-hydroxyacetofenone the PECs exceed or equal the PNEC. The Finnish model — showing RCRs of 1.4-1289, when assuming an additional dilution factor of 10 for the STP effluent to the recipient surface water — may be more realistic as it includes process temperature dependent hydrolysis and degradation. Therefore, the high RCRs calculated by USES appear to have a realistic element, although it should be noted that the Finnish peak value of 12886 refers to an atypical — though realistic — plant with a very high waste water volume. As sorption data are not available the refined risk assessment may be hampered (for the current calculations the sorption coefficients are based on the log K_{ow})

The reliability of the ecotoxicity data on which the PNEC is based and the reliability of the extrapolated sorption data — as explained above — may be doubted. Therefore CTB requires as conditions for reregistration in the Netherlands in 2002 the following environmental data: -1- a (semi) field study on the effects to aquatic organisms -2- a biodegradation study in a water/sediment system -3- reliable ecotoxicity tests with algae, crustaceans and fish -4- a study on the sorption to suspended sediment and -5- a bioaccumulation study with fish. These requirements fit with the results of the refined risk assessment: high risks may occur. However, the refined assessment also makes clear that more detailed data on actual concentrations *c.g.* emissions from paper mills will be very helpful for a proper exposure analysis as well.

6

CAS no. 2682-20-4

2-methyl-4-isothiazolin-3-one

Syn.: 2-methyl-2H-isothiazol-3-one; 3(2H)-isothiazole, 2-methyl; methylisothiazoline

molecular weight	vapour pressure	water solubility	log K _{ow}
(-)	(Pa)	(mg/litre)	(-)
114.0	4.1*	1000	-0.83*

* EPIWIN estimates (vapour pressure at 25 °C).

AQUATIC ENVIRONMENTAL/ECOTOXICOLOGICAL ENDPOINTS							
DT ₅₀ (hydrolysis)	DT ₅₀ (photolysis in water)	DT ₅₀ (biodegradation in water)	EC ₅₀ (STP microbes)	EC ₅₀ (algae)	E(L)C ₅₀ (crustaceans)	LC ₅₀ (fish)	BCF (fish)
(days)	(days)	(days)	(mg/litre)	(mg/litre)	(mg/litre)	(mg/litre)	(-)
30	-	0.38*	1165	0.01**	0.18***	0.07-0.86***	-

* EPIWIN indicates the probability of rapid biodegradation of 0.7-0.8.

** refers to the a.i. in a product with 5-chloro-2-methyl-4-isothiazoline-3-one as well.

*** refers to the a.i. of 14-90% products that contain 5-chloro-2-methyl-4-isothiazoline-3-one as well. A 21-d NOEC for crustaceans of 0.1 mg a.i./litre. MATCs for crustaceans and fish were 0.13 and 0.035 mg a.i./litre, respectively (EPA, 1998).

PRODUCT TYPE & EMISSIONS						
PRODUCT TYPE	SHORT DESCRIPTION	EMISSIONS EXPECTED TO*,**				
(code)		STP	SURFACE WATER	SEDI-MENT	SOIL	OUTDOOR AIR
8.1	Wood preservative (industrial)	EQ ¹	EQ ²	EQ ³	EQ ⁴	N ⁵
11	Liquid-cooling system preservative	N ¹	Y ²	EQ ³	EQ ⁴	N ⁵
12.1	Slimeicide (paper industry)	Y ¹	Y ²	EQ ³	EQ ⁴	N ⁵

* for notes: see table on preliminary environmental risk assessment in Mensink (1999).

** Y = yes; N = no; EQ = equivocal.

RCRs INITIAL & REFINED RISK ASSESSMENT & HAZARD GROUP					
PRODUCT TYPE	SHORT DESCRIPTION	RCR*			HAZARD GROUP
(code)		INITIAL	LOWEST	HIGHEST	
8.1	Wood preservative	4.3	0.0001	26	HAZARDOUS APPLICATION
11	Liquid-cooling system preservative	243	270	2179	VERY HAZARDOUS APPLICATION
12.1	Slimeicide (paper industry)	5657	0.0029	37	HAZARDOUS APPLICATION

* for further details see Appendix 3, p. 90, 104 & 110.

REFINED ENVIRONMENTAL RISK ASSESSMENT

Refined risk assessment shows that 2-methyl-4-isothiazolin-3-one is a (very) hazardous substance, independent of the type of use. It does not hydrolyse, but it is assumed to be readily biodegradable in an STP. The high partition coefficients for sediment and suspended matter substantiates appear to be conflicting with its high water solubility.

Refined risk assessment shows that as a liquid-cooling system preservative the RCRs are higher compared with the initial risk assessment (the same was found *e.g.* for 2,2-dibromo-3-nitropropionamide) — in spite of introducing more realistic data on hydrolysis and degradation. This may imply that for water-cooling biocides the “default” assumptions of the initial risk assessment rather refer to typical than to atypical conditions. This appears to be confirmed by a few measurements of 2-methyl-4-isothiazolin-3-one in the blow-down of Dutch electricity plants with an RCR of the parent compound of 486-2000 (based on a measured concentration of 340-1400 µg/litre; Baltus *et al.*, 1999), a range that coincides with the RCR range of the refined risk assessment. It should be noted, however, that these RCRs refer to the blow-down before physical treatment or discharge on an STP, and therefore the final amounts of 2-methyl-4-isothiazolin-3-one in the recipient surface water — and thus the corresponding RCRs — are expected to be lower. The hazardousness of 2-methyl-4-isothiazolin-3-one for the aquatic environment was also reported by Baltus *et al.* (1999). They stated that in toxicity tests isothiazolines containing effluent of 3 facilities was acutely toxic to algae, crustaceans and fish.

When used as a slimicide, the RCRs of the initial assessment are lower than those of the refined assessment: only the adjusted USES scenario indicates that the substance is hazardous, whereas the other scenarios indicate that the substance is non-hazardous. There is no clear explanation for these differences. However, the Finnish model — showing RCRs of 0.0003-1,3 when assuming an additional dilution factor of 10 for the STP effluent to the recipient water — may be more realistic as it includes process temperature dependent hydrolysis and degradation. This indicates that hazards may turn out better than expected.

Monitoring in STP effluent of large paper factories in Sweden en Finland (32500 - 45000 m³/d) showed concentrations of c. 13 and c. 4 µg/litre, respectively. These concentrations probably refer to the sum of 2-methyl-4-isothiazolin-3-one and 5-chloro-2-methyl-4-isothiazoline-3-one. Assuming a dilution factor of 10 for the recipient water (worst-case), then these actual concentrations show the same order of magnitude as most model outcomes, except USES. This may be an extra indication that the worst-case scenarios of USES give PECs for atypical sites only — if realistic at all. It should be noted, however, that there were only two measurements in three paper plants with different STPs.

The use of 2-methyl-4-isothiazolin-3-one as a wood preservative is for all scenarios (impregnation facilities, direct leaching from sheet piles into surface water) not hazardous for the aquatic environment, except when it is assumed that a relatively large amount leaches from the wood. At least under marine conditions, however, these large amounts could indeed be leached: the EPA (1998) found that in pine wood blocks in artificial sea water 84% of the impregnated amount leached within 28 days into the water. In this leaching test the wood was impregnated by both 5-chloro-2-methyl-4-isothiazolin-3-one and 2-methyl-4-isothiazolin-3-one, so the leaching percentage refers to the compound sum.

The use of 2-methyl-4-isothiazolin-3-one (and 5-chloro-2-methyl-4-isothiazolin-3-one which is a co-substance of products with 2-methyl-4-isothiazolin-3-one) is legally restricted to recirculating systems. This combination of substances should only be used with the authorisation of the local authorities of qualitative water management.

CONTINUED ON NEXT PAGE

REFINED ENVIRONMENTAL RISK ASSESSMENT

The Board for the Authorisation of Pesticides has not yet verified whether the dossiers for reregistration of both substances are complete (reference date 27-03-2000).

7

CAS no. 7166-19-0

bromonitrostyrene

Syn.: (2-bromo-2-nitrovinyl)benzene; benzene, (2-bromo-2-nitroethenyl)-

molecular weight	vapour pressure	water solubility	log K _{ow}
(-)	(Pa)	(mg/litre)	(-)
228.0	0.090*	127*	2.3*

* EPIWIN estimate (vapour pressure and water solubility at 25 °C).

AQUATIC ENVIRONMENTAL/ECOTOXICOLOGICAL ENDPOINTS							
DT ₅₀ (hydrolysis)	DT ₅₀ (photolysis in water)	DT ₅₀ (biodegradation in water)	EC ₅₀ (STP microbes)	EC ₅₀ (algae)	E(L)C ₅₀ (crustaceans)	LC ₅₀ (fish)	BCF (fish)
(days)	(days)	(days)	(mg/litre)	(mg/litre)	(mg/litre)	(mg/litre)	(-)
-	-	*	-	1.8**	0.38	0.11-0.24	-

* EPIWIN indicates a probability of rapid biodegradation of 0.05-0.7.

** refers to the a.i. of a 9.2% product. However, this product also contains another a.i. besides bromonitrostyrene.

PRODUCT TYPE & EMISSIONS						
PRODUCT TYPE (code)	SHORT DESCRIPTION	EMISSIONS EXPECTED TO*,**				
		STP	SURFACE WATER	SEDI-MENT	SOIL	OUTDOOR AIR
11 12.1	Liquid-cooling system preservative Slimicide (paper industry)	N ¹ EQ ¹	EQ ² EQ ²	EQ ³ EQ ³	EQ ⁴ EQ ⁴	N ⁵ N ⁵

* for notes: see table on preliminary environmental risk assessment in Mensink (1999).

** Y = yes; N = no; EQ = equivocal.

REFINED ENVIRONMENTAL RISK ASSESSMENT
All registrations with bromonitrostyrene have been withdrawn from the market. Therefore no further refined risk assessment is needed.

8

CAS no. 1085-98-9

dichlofluanide

molecular weight	vapour pressure	water solubility	log K _{ow}
(-)	(Pa)	(mg/litre)	(-)
333.2	1.6×10 ⁻⁵	1.3	2.7*

* EPIWIN estimate.

AQUATIC ENVIRONMENTAL/ECOTOXICOLOGICAL ENDPOINTS*							
DT ₅₀ (hydrolysis)	DT ₅₀ (photolysis in water)	DT ₅₀ (biodegradation in water)	EC ₅₀ (STP microbes)	EC ₅₀ (algae)	E(L)C ₅₀ (crustaceans)	LC ₅₀ (fish)	BCF (fish)
(days)	(days)	(days)	(mg/litre)	(mg/litre)	(mg/litre)	(mg/litre)	(-)
-	-	*	-	-	-	0.05-0.12	-

* The MPC for dichlofluanide was reported to be 30 µg/litre (CUWVO/CIW, 1999).

**EPIWIN indicates a probability of rapid biodegradation of 0.005-0.3.

PRODUCT TYPE & EMISSIONS						
PRODUCT TYPE	SHORT DESCRIPTION	EMISSIONS EXPECTED TO*,**				
(code)		STP	SURFACE WATER	SEDI-MENT	SOIL	OUTDOOR AIR
6.3	In-can preservative (others)	Y ¹	EQ ²	EQ ³	EQ ⁴	N ⁵
8.1	Wood preservative (industrial)	EQ ¹	EQ ²	EQ ³	EQ ⁴	N ⁵
21	Antifouling product	N ¹	EQ ²	EQ ³	N ⁴	N ⁴

* for notes: see table on preliminary environmental risk assessment in Mensink (1999).

** Y = yes; N = no; EQ = equivocal.

RCRs INITIAL & REFINED RISK ASSESSMENT & HAZARD GROUP					
PRODUCT TYPE	SHORT DESCRIPTION	RCR*			HAZARD GROUP
(code)		INITIAL	LOWEST	HIGHEST	
6.3	In-can preservative (others)	274	N.D.**	N.D.	NOT DETERMINED
8.1	Wood preservative (industrial)	6.4	0.011	0.021	NON-HAZARDOUS APPLICATION
21	Antifouling product	640	N.D.	N.D.	NOT DETERMINED

* for further details see Appendix 3, p. 105.

** N.D. is not determined.

REFINED ENVIRONMENTAL RISK ASSESSMENT

Refined risk assessment shows that dichlofluanide is a non-hazardous substance, when used as a wood preservative for impregnation. The lower RCRs in the refined risk assessment — compared with the initial risk assessment — are not so much due to a different exposure analysis, but to a different effect analysis: an *ad hoc* MPC of 30 µg/litre (CUWVO/CIW, 1999) was used instead of a much lower — but less well substantiated — PNEC of 0.05 µg/litre (Mensink, 1999). Worst-case assumptions with respect to hydrolysis and degradation need not be adjusted as PECs are already below this PNEC.

No refined risk assessments were performed for dichlofluanide as an in-can preservative or as an antifouling product as these did not belong to the substance-specific applications with the highest abundance.

Dichlofluanide has been reported as a hormonal active substance in the environment in a review of the German Umweltbundesamt (Schramm *et al.*, 1996). However, a concentration range for which this “hormonal activity” was found, was not reported. Probably, this hormonal activity is not taken into account in the abovementioned PEC/PNEC approach.

9

CAS no. 50-00-0

formaldehyde

molecular weight	vapour pressure	water solubility	log K _{ow}
(-)	(Pa)	(mg/litre)	(-)
30.0	173,000*	1000**	0.35***

* EPIWIN estimate (at 25 °C).

** actually readily soluble.

*** experimental value from EPIWIN database.

AQUATIC ENVIRONMENTAL/ECOTOXICOLOGICAL ENDPOINTS							
DT ₅₀ (hydrolysis)	DT ₅₀ (photolysis in water)	DT ₅₀ (biodegradation in water)	EC ₅₀ (STP microbes)	EC ₅₀ (algae)	E(L)C ₅₀ (crustaceans)	LC ₅₀ (fish)	BCF (fish)
(days)	(days)	(days)	(mg/litre)	(mg/litre)	(mg/litre)	(mg/litre)	(-)
-	-	1* **	>25-450	0.3-15	1.0**-5.8***	6.7-7200**	-

* EPIWIN indicates a probability of rapid biodegradation of 1.0.

** Source: IPCS (1989)⁹.

*** Tišler & Zagorc-Konšan (1996).

PRODUCT TYPE & EMISSIONS						
PRODUCT TYPE	SHORT DESCRIPTION	EMISSIONS EXPECTED TO*,**				
(code)		STP	SURFACE WATER	SEDI-MENT	SOIL	OUTDOOR AIR
2.1	Public health area (medical equipment)	EQ ¹	EQ ²	N ³	N ³	EQ ³
2.4	Public health area (accommodation for man)	Y ¹	EQ ²	N ³	N ³	EQ ³
2.6	Public health area (chemical toilet)	EQ ¹	EQ ²	N ³	N ³	EQ ³
2.10	Public health area (other)	EQ ¹	EQ ²	N ³	N ³	EQ ³
4	Food and feed area	EQ ¹	EQ ²	N ³	N ³	EQ ³

* for notes: see table on preliminary environmental risk assessment in Mensink (1999).

** Y = yes; N = no; EQ = equivocal.

⁹ IPCS (1989) Formaldehyde. EHC 89, IPCS/WHO, Geneva.

RCRs INITIAL & REFINED RISK ASSESSMENT & HAZARD GROUP					
PRODUCT TYPE	SHORT DESCRIPTION	RCR*			HAZARD GROUP
(code)		INITIAL	LOWEST	HIGHEST	
2.1	Public health area (medical equipment)	N.D.**	8.3	8.3	“DISPUTABLY”HAZARDOUS APPLICATION
2.4	Public health area (accommodation for man)	1.5	0.56	0.83	NON-HAZARDOUS APPLICATION
2.6	Public health area (chemical toilet)	N.D.	N.D.	N.D.	NOT DETERMINED
2.10	Public health area (other)	N.D.	0.01	1.6	“DISPUTABLY” HAZARDOUS APPLICATION
4	Food and feed area	N.D.	N.D.	N.D.	“DISPUTABLE” APPLICATION

* for further details see Appendix 3, p. 97.

** N.D. is not determined.

REFINED ENVIRONMENTAL RISK ASSESSMENT
<p>Refined risk assessment shows that for most scenarios formaldehyde is a non-hazardous substance, when used as a wood preservative and when impregnating. Only when used for disinfecting medical equipment and for washing hospital laundry in washing streets the PECs are assumed to exceed the PNEC (max. 8.3 and 1.6 times, respectively). This in spite of its rapid degradation in STPs. No RCRs are determined for the use of formaldehyde in chemical toilets and in the food and feed area as no appropriate models are available.</p> <p>Formaldehyde in water tends to polymerise, and this transformation product may behave different in the environment. No data on this issue are available.</p>

10

CAS no. 3567-25-7

sulcofuron

Syn.: sulcofenuron

molecular weight	vapour pressure	water solubility	log K _{ow}
(-)	(Pa)	(mg/litre)	(-)
522.2	4.0×10 ⁻²⁰ *	20,000**	1.8

* EPIWIN estimate at 25 °C.

** EPIWIN indicates a water solubility at 25 °C of 11 mg/litre.

However, this refers to the sodium salt of sulcofuron.

AQUATIC ENVIRONMENTAL/ECOTOXICOLOGICAL ENDPOINTS							
DT ₅₀ (hydrolysis)	DT ₅₀ (photolysis in water)	DT ₅₀ (biodegradation in water)	EC ₅₀ (STP microbes)	EC ₅₀ (algae)	E(L)C ₅₀ (crustaceans)	LC ₅₀ (fish)	BCF (fish)
(days)	(days)	(days)	(mg/litre)	(mg/litre)	(mg/litre)	(mg/litre)	(-)
-	-	*	-	-	9.5	7	-

*EPIWIN indicates a probability of rapid biodegradation of 0.0.

PRODUCT TYPE & EMISSIONS						
PRODUCT TYPE	SHORT DESCRIPTION	EMISSIONS EXPECTED TO*,**				
(code)		STP	SURFACE WATER	SEDI-MENT	SOIL	OUTDOOR AIR
9.1	Fibre/polymer preservative (textile)	Y ¹	N ¹ ?	N ¹ ?	EQ ¹	N ¹

* for notes: see table on preliminary environmental risk assessment in Mensink (1999).

** Y = yes; N = no; EQ = equivocal.

RCRs INITIAL & REFINED RISK ASSESSMENT & HAZARD GROUP					
PRODUCT TYPE	SHORT DESCRIPTION	RCR			HAZARD GROUP
(code)		INITIAL	LOWEST	HIGHEST	
9.1	Fibre/polymer preservative (textile)	3.3	N.D.*	N.D.	UNKNOWN

* N.D. is not determined.

REFINED ENVIRONMENTAL RISK ASSESSMENT

No refined risk assessment was performed as sulcofuron was not among the substance-specific applications with the highest abundance. However, it should be noted, that high amounts of sulcofuron may currently be used. The most recent estimate of its yearly use of 888,000 kg goes back to 1992.

11

CAS no. 1314-13-2

zinc oxide

molecular weight	vapour pressure	water solubility	log K _{ow}
(-)	(Pa)	(mg/litre)	(-)
81.4	-	2	-

AQUATIC ENVIRONMENTAL/ECOTOXICOLOGICAL ENDPOINTS							
DT ₅₀ (hydrolysis)	DT ₅₀ (photolysis in water)	DT ₅₀ (biodegradation in water)	EC ₅₀ (STP microbes)	EC ₅₀ (algae)	E(L)C ₅₀ (crustaceans)	LC ₅₀ (fish)	BCF (fish)
(days)	(days)	(days)	(mg/litre)	(mg/litre)	(mg/litre)	(mg/litre)	(-)
-	-	-	-	*	**	0.09***	6

* NOEC (algae) is 0.015-0.7 mg/litre.

** NOEC (crustaceans) is 0.037-0.075 mg/litre.

*** NOEC (fish) is 0.026-0.030 mg/litre.

PRODUCT TYPE & EMISSIONS						
PRODUCT TYPE	SHORT DESCRIPTION	EMISSIONS EXPECTED TO*,**				
(code)		STP	SURFACE WATER	SEDI-MENT	SOIL	OUTDOOR AIR
21	Antifouling product	N ¹	EQ ²	EQ ²	N ³	N ⁴

* for notes: see table on preliminary environmental risk assessment in Mensink (1999).

** Y = yes; N = no; EQ = equivocal.

REFINED ENVIRONMENTAL RISK ASSESSMENT
<p>No refined risk assessment was performed as zinc oxide was not among the substance-specific applications with the highest abundance.</p> <p>The pattern of environmental behaviour — when zinc oxide is used as antifouling — is unclear. Due to the very slight water solubility zinc oxide is primarily expected to sorb to suspended particles. The EPA (1992a) concluded that zinc salts — as zinc oxide — are not expected to contribute to the increase of free zinc oxide (Zn²⁺), the actual source of toxicity to aquatic organisms. Therefore the EPA stated that zinc salts — as zinc oxide — are not likely to cause unreasonable effects in the environment. However, the EPA did not focus on the particular use of zinc oxide as an antifouling.</p>

12

CAS no. 2527-57-3

2,2-dithio-bis-benzamide

syn.: benzamide, 2,2-dithiobis

molecular weight	vapour pressure	water solubility	log K _{ow}
(-)	(Pa)	(mg/litre)	(-)
304.4	5×10 ⁻¹⁰ *	298*	0.33*

* EPIWIN estimates (vapour pressure and water solubility at 25 °C).

AQUATIC ENVIRONMENTAL/ECOTOXICOLOGICAL ENDPOINTS							
DT ₅₀ (hydrolysis)	DT ₅₀ (photolysis in water)	DT ₅₀ (biodegradation in water)	EC ₅₀ (STP microbes)	EC ₅₀ (algae)	E(L)C ₅₀ (crustaceans)	LC ₅₀ (fish)	BCF (fish)
(days)	(days)	(days)	(mg/litre)	(mg/litre)	(mg/litre)	(mg/litre)	(-)
-	-	*	-	-	-	-	-

*EPIWIN indicates a probability of rapid biodegradation of 1.0.

PRODUCT TYPE & EMISSIONS						
PRODUCT TYPE	SHORT DESCRIPTION	EMISSIONS EXPECTED TO*,**				
(code)		STP	SURFACE WATER	SEDI-MENT	SOIL	OUTDOOR AIR
6.3	In-can preservative, others	EQ ¹	EQ ²	EQ ³	EQ ⁴	N ⁵
12.1	Slimicide (paper industry)	EQ ¹	EQ ²	EQ ³	EQ ⁴	N ⁵

* for notes: see table on preliminary environmental risk assessment in Mensink (1999).

** Y = yes; N = no; EQ = equivocal.

RCRs INITIAL & REFINED RISK ASSESSMENT & HAZARD GROUP					
PRODUCT TYPE	SHORT DESCRIPTION	RCR			HAZARD GROUP
(code)		INITIAL	LOWEST	HIGHEST	
6.3	In-can preservative, others	N.D.*	N.D.	N.D.	UNKNOWN
12.1	Slimicide (paper industry)	N.D.	N.D.	N.D.	UNKNOWN

* N.D. is not determined (e.g. as ecotoxicity data are lacking).

REFINED ENVIRONMENTAL RISK ASSESSMENT

There is conflicting information on the actual use rate of 2,2-dithio-bis-benzamide in the Netherlands. Therefore, the emission patterns are unclear, and so, substantial emissions to STPs and, possibly, to surface waters and their corresponding sediments cannot be excluded, particularly when used in paper industries. Only EPIWIN data are available.

No refined risk assessment was performed for 2,2-dithio-bis-benzamide as no ecotoxicity data could be found and — as an in-can preservative— it was not among the substance-specific applications with the highest abundance. When used as a slimicide even an initial risk assessment can not be performed because the yearly use rate is not available, whereas this data is required for a calculation with USES 2.0. Assuming ready biodegradability — which seems to be most likely, although there are no empirical data for substantiation —, and assuming a max. concentration in process water of 40 mg/litre, as was reported to be a general maximum for chemicals used in the paper industry (ECB, 1996), and also assuming a K_{oc} of 2100 dm³/kg — based on log K_{ow} — the PEC is 510 µg/litre.

CTB stated on 15-10-1999 that PROXEL CF — a product that was not reported in Mensink (1999) as it was erroneously indexed in the CTB pesticide data base — that contains a.o. 2,2-dithio-bis-benzamide was only registered as a preservative for industrial products on a water base. CTB stated on 11-06-1999 that for another product with 2,2-dithio-bis-benzamide PROXEL GXL — to be used in water-based products or as a slimicide — additional environmental data should be submitted by the registrant as prerequisites for reregistration: with respect to 2,2-dithio-bis-benzamide these data include chronic toxicity to crustaceans, chronic toxicity to fish (28-days juvenile growth test) and chronic toxicity to the sediment dwelling larvae of *Chironomus*.

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CAS no. unknown

4-chloro-3-methyl-phenolate sodium

syn.: 4-chloro-3-methyl-sodiumphenoxide

molecular weight	vapour pressure	water solubility	log K _{ow}
(-)	(Pa)	(mg/litre)	(-)
130.1	-	-	-

AQUATIC ENVIRONMENTAL/ECOTOXICOLOGICAL ENDPOINTS							
DT ₅₀ (hydrolysis)	DT ₅₀ (photolysis in water)	DT ₅₀ (biodegradation in water)	EC ₅₀ (STP microbes)	EC ₅₀ (algae)	E(L)C ₅₀ (crustaceans)	LC ₅₀ (fish)	BCF (fish)
(days)	(days)	(days)	(mg/litre)	(mg/litre)	(mg/litre)	(mg/litre)	(-)
-	-	-	-	-	-	-	-

PRODUCT TYPE & EMISSIONS						
PRODUCT TYPE (code)	SHORT DESCRIPTION	EMISSIONS EXPECTED TO*,**				
		STP	SURFACE WATER	SEDI-MENT	SOIL	OUTDOOR AIR
6.3	In-can preservative (others)	EQ ¹	N	N	N	N

* for notes: see table on preliminary environmental risk assessment in Mensink (1999).

** Y = yes; N = no; EQ = equivocal.

RCRs INITIAL & REFINED RISK ASSESSMENT & HAZARD GROUP					
PRODUCT TYPE (code)	SHORT DESCRIPTION	RCR			HAZARD GROUP
		INITIAL	LOWEST	HIGHEST	
6.3	In-can preservative, others	N.D.*	N.D.	N.D.	NOT DETERMINED

- N.D. is not determined (e.g. as ecotoxicity data are lacking)

REFINED ENVIRONMENTAL RISK ASSESSMENT

4-chloro-3-methyl-phenolate sodium is the sodium salt of 4-chloro-3-methylphenol (see also Mensink, 1999). A more exhaustive literature search revealed no CAS number, and no physicochemical, environmental, or ecotoxicological data. As no pKa value is available of 4-chloro-3-methylphenol¹⁰, it is difficult to state whether the phenol or the phenolate species prevail at *e.g.* pH 7. In case the phenol species prevail, additional data on the salt may not be necessary. The industry should clarify this issue. Until then, the data available are not considered sufficient for performing an initial risk assessment. Such a preliminary risk assessment, however, is considered necessary as environmental emissions cannot be excluded, when used as an in-can preservative. On the other hand, VNCI (1993) estimated a total use rate of 4-chloro-3-methyl-phenolate sodium in 1992 of 93 kg. If this estimate is correct, substantial local emissions to the environment can probably be neglected. However, it is not clear, whether the VNCI estimate is really representative for the actual use.

As initial risk assessment was not possible, refined risk assessment was — of course — also not possible.

¹⁰ *E.g.* no pKa is reported in: Mackay D., Shiu W.Y. and Ma K.C. (1995) Illustrated Handbook of Physical-Chemical Properties and Environmental Fate for Organic Chemicals. Vol. IV. CRC Lewis Publishers, Boca Raton, New York, London, Tokyo.

5-chloro-2-methyl-4-isothiazolin-3-one

molecular weight	vapour pressure	water solubility	log K _{ow}
(-)	(Pa)	(mg/litre)	(-)
149.6	0.72*	1.5×10 ⁵ *	-0.34*

* EPIWIN estimates (vapour pressure and water solubility at 25 °C).

AQUATIC ENVIRONMENTAL/ECOTOXICOLOGICAL ENDPOINTS							
DT ₅₀ (hydrolysis)	DT ₅₀ (photolysis in water)	DT ₅₀ (biodegradation in water)	EC ₅₀ (STP microbes)	EC ₅₀ (algae)	E(L)C ₅₀ (crustaceans)	LC ₅₀ (fish)	BCF (fish)
(days)	(days)	(days)	(mg/litre)	(mg/litre)	(mg/litre)	(mg/litre)	(-)
22	30	0.71*	1165**	0.01**	0.18***	<0.27-0.30****	-

* EPIWIN indicates a probability of rapid biodegradation of 0.3-0.6.

** refers to the a.i. in a product with 2-methyl-4-isothiazoline-3-one as well.

*** refers to the products that contain 2-methyl-4-isothiazoline-3-one as well. A 21-d NOEC for crustaceans was 0.1 mg a.i./litre.

**** refers to a product with 2-methyl-4-isothiazoline-3-one as well. A 14-d NOEC was 0.05 mg/litre.

PRODUCT TYPE & EMISSIONS						
PRODUCT TYPE	SHORT DESCRIPTION	EMISSIONS EXPECTED TO*,**				
(code)		STP	SURFACE WATER	SEDI-MENT	SOIL	OUTDOOR AIR
8.1	Wood preservative (industrial)	EQ ¹	EQ ²	EQ ³	EQ ⁴	N ⁵
11	Liquid-cooling system preservative	N ¹	Y ²	EQ ³	EQ ⁴	N ⁵
12.1	Slimeicide (paper industry)	Y ¹	Y ²	EQ ³	EQ ⁴	N ⁵

* for notes: see table on preliminary environmental risk assessment in Mensink (1999).

** Y = yes; N = no; EQ = equivocal.

RCRs INITIAL & REFINED RISK ASSESSMENT & HAZARD GROUP					
PRODUCT TYPE	SHORT DESCRIPTION	RCR*			HAZARD GROUP
(code)		INITIAL	LOWEST	HIGHEST	
8.1	Wood preservative (industrial)	0.17	0.0001	24	HAZARDOUS APPLICATION
11	Liquid-cooling system preservative	85	265	1971	VERY HAZARDOUS APPLICATION
12.1	Slimeicide (paper industry)	2000	0.0025	25	HAZARDOUS APPLICATION

* for further details see Appendix 3, p. 91, 106 & 111.

REFINED ENVIRONMENTAL RISK ASSESSMENT

Refined risk assessment shows that 5-chloro-2-methyl-4-isothiazolin-3-one is a hazardous or very hazardous substance, when used as a wood preservative and a slimicide, or as a liquid-cooling system, respectively. It does not hydrolyse at room temperature — which may be the reason for its relative persistence in *e.g.* cooling-water systems (person. communic. Baltus (RIZA) to RIVM) — but it is assumed to be readily biodegradable in an STP. 2-methyl-4-isothiazolin-3-one is probably the first major metabolite.

Refined risk assessment shows that as a liquid-cooling system preservative the RCRs are higher compared with the initial risk assessment (the same was found for *e.g.* 2,2-dibromo-3-nitropropionamide and 2-methyl-4-isothiazolin-3-one) — in spite of introducing more realistic data and degradation. This may imply that for cooling-water biocides the “default” assumptions of the initial risk assessment rather refer to typical than to atypical conditions. This appears to be confirmed by a few measurements of 5-chloro-2-methyl-4-isothiazolin-3-one in the blow-down of Dutch electricity plants with an RCR of the parent compound of 430-1200 (based on a measured concentration of 860-2400 µg/litre; Baltus *et al.*, 1999), a range that coincides with the RCR range of the refined risk assessment. It should be noted, however, that these RCRs refer to the blow-down before physical treatment or discharge on an STP, and therefore the final amounts of 2-methyl-4-isothiazolin-3-one in the recipient surface water — and thus the corresponding RCRs — are expected to be lower. The hazardousness of 5-chloro-2-methyl-4-isothiazolin-3-one for the aquatic environment was also reported by Baltus *et al.* (1999). They stated that in toxicity tests isothiazolines containing effluent of 3 facilities was acutely toxic to algae, crustaceans and fish.

When used as a slimicide, the RCRs of the initial assessment are lower than those of the refined assessment: the adjusted USES scenario and one Finnish scenarios — for an atypical paper mill with a very high waste water volume — still exceed a PEC/PNEC of 1. The other Finnish and Swedish scenarios indicate that the substance is not hazardous. There is no clear explanation for these differences. However, the Finnish model — showing RCRs of 0.003-9.9, when assuming an additional dilution factor of 10 for the STP effluent to the recipient surface water — may be more realistic as it includes process temperature dependent hydrolysis and degradation. This appears to indicate that only under extreme conditions — very large plants, very high dosages — hazards can be expected.

Monitoring in STP effluent of large paper factories in Sweden and Finland (32500 - 45000 m³/d) showed concentrations of *c.* 13 and *c.* 4 µg/litre, respectively. These concentrations probably refer to the sum of 2-methyl-4-isothiazolin-3-one and 5-chloro-2-methyl-4-isothiazolin-3-one. Assuming a dilution factor of 10 for the recipient water (worst-case), then these actual concentrations are below the PNEC, indicating no hazards for the aquatic environment. This appears to coincide with the notion — as stated above — that under more typical conditions, hazards are not expected. It should be noted, however, that there were only two measurements in three paper plants with different STPs. Therefore the validity of the conclusion that under typical conditions the effects on aquatic organisms turn out to be better than expected is limited.

The use of 5-chloro-2-methyl-4-isothiazolin-3-one as a wood preservative is for all scenarios (impregnation facilities, direct leaching from sheet piles into surface water) not hazardous for the aquatic environment, except when it is assumed that a relatively large amount leaches from the wood. At least under marine conditions, however, these large amounts could indeed be leached: the EPA (1998) found that in pine wood blocks in artificial sea water 84% of the impregnated amount leached within 28 days into the water. In this leaching test the wood was impregnated by both 5-chloro-2-methyl-4-isothiazolin-3-one and 2-methyl-4-isothiazolin-3-one, so the leaching percentage refers to the compound sum.

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REFINED ENVIRONMENTAL RISK ASSESSMENT

The use of 5-chloro-2-methyl-4-isothiazolin-3-one (and 2-methyl-4-isothiazolin-3-one which is a co-substance of products with 5-chloro-2-methyl-4-isothiazolin-3-one) is legally restricted to recirculating systems. This combination of substances should only be used with the authorisation of the local authorities for qualitative water management.

The Board for the Authorisation of Pesticides has not yet verified whether the dossiers for reregistration of both substances are complete (reference date 27-03-2000).

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CAS no. 1192-52-5

5-oxo-3,4-dichloro-1,2-dithiol

(syn.: DARACIDE 7816)

molecular weight	vapour pressure	water solubility	log K _{ow}
(-)	(Pa)	(mg/litre)	(-)
186.0	1.5-1.7*	500*	1.8**

* at 25 °C.

** EPIWIN estimate.

AQUATIC ENVIRONMENTAL/ECOTOXICOLOGICAL ENDPOINTS							
DT ₅₀ (hydrolysis)	DT ₅₀ (photolysis in water)	DT ₅₀ (biodegradation in water)	EC ₅₀ (STP microbes)	EC ₅₀ (algae)	E(L)C ₅₀ (crustaceans)	LC ₅₀ (fish)	BCF (fish)
(days)	(days)	(days)	(mg/litre)	(mg/litre)	(mg/litre)	(mg/litre)	(-)
4.3	0.1	0.2*	-	-	0.36	0.014-0.018	-

* EPIWIN indicates a probability of rapid biodegradation of 0.03-0.4.

PRODUCT TYPE & EMISSIONS						
PRODUCT TYPE	SHORT DESCRIPTION	EMISSIONS EXPECTED TO*,**				
(code)		STP	SURFACE WATER	SEDI-MENT	SOIL	OUTDOOR AIR
12.1	Slimicide (paper industry)	EQ ¹	EQ ²	EQ ³	EQ ⁴	EQ ⁵

* for notes: see table on preliminary environmental risk assessment in Mensink (1999).

** Y = yes; N = no; EQ = equivocal.

RCRs INITIAL & REFINED RISK ASSESSMENT & HAZARD GROUP					
PRODUCT TYPE	SHORT DESCRIPTION	RCR*			HAZARD GROUP
(code)		INITIAL	LOWEST	HIGHEST	
12.1	Slimicide (paper industry)	281,429	0.00036	1500	VERY HAZARDOUS APPLICATION

* for further details see Appendix 3, p. 93.

REFINED ENVIRONMENTAL RISK ASSESSMENT	
<p>Refined risk assessment shows that 5-oxo-3,4-dichloro-1,2-dithiol is a very hazardous substance, when used as a slimicide. However, the RCR range is enormous, indicating that conditions may prevail with no hazards when using 5-oxo-3,4-dichloro-1,2-dithiol. The fact that USES 2.0 gives an RCR of 1500 is not unexpectedly in view of the assumption of no hydrolysis or degradation (as these data were not available then). The same calculation but now</p>	

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REFINED ENVIRONMENTAL RISK ASSESSMENT

with more realistic data on hydrolysis and degradation still indicates a PEC that substantially exceeds the PNEC (RCR of 71). It is also surprising that the Finnish scenario with an atypically high waste water volume has a low RCR of 0.0054, whereas a less large plant has a much higher RCR of 57 (for both an additional dilution factor of 10 is used conform USES 2.0). There is no clear explanation: the input data for $DT_{50,biodeg,wat/sed}$, for $DT_{50,biodeg,STP}$ and $DT_{50,hydrol}$ are *e.g.* the same for both scenarios. Probably the application rate is erroneously reported in WG/GA. In conclusion: a more realistic approach still gives PECs exceeding the PNEC for at least one of the Dutch, Swedish or Finnish scenarios. However, refined risk assessment reduces the RCR of the initial risk assessment substantially, although it is difficult to compare the models with each other. Whereas for other substances the Finnish approach seems to be more realistic — due to the introduction of process temperature dependent hydrolysis and degradation rates rather than fixed values — this does not seem to be the case here. There are no monitoring data available that might have given an answer to these questions.

Major metabolites of 5-oxo-3,4-dichloro-1,2-dithiol due to photolysis is chloranil (syn.: hydroquinone): an active ingredient itself that hydrolyses at comparable rates as the parent compound; it can also react with organic matter. Hydrolytical metabolites are two heterocyclic carboxylic acids, thiol-acid and keto-acid.

Finally it should be noted that the registration for the only product with 5-oxo-3,4-dichloro-1,2-dithiol has been expired since 01-12-98. There is an additional period until 01-07-2000 that carry-overs can be sold.

arsenic pentoxide

molecular weight	vapour pressure	water solubility	log K _{ow}
(-)	(Pa)	(mg/litre)	(-)
229.8	3.8×10 ⁻⁸ *	40,000*	-

* EPIWIN estimate at 25 °C (arbitrary value as EPIWIN is actually not appropriate for anorganic chemicals).

AQUATIC ENVIRONMENTAL/ECOTOXICOLOGICAL ENDPOINTS							
DT ₅₀ (hydrolysis)	DT ₅₀ (photolysis in water)	DT ₅₀ (biodegradation in water)	EC ₅₀ (STP microbes)	EC ₅₀ (algae)	E(L)C ₅₀ (crustaceans)	LC ₅₀ (fish)	BCF (fish)
(days)	(days)	(days)	(mg/litre)	(mg/litre)	(mg/litre)	(mg/litre)	(-)
-	-	-	-	*	*	*	-

* An MPA of 24 µg As/litre has been derived for aquatic organisms by Crommentuijn *et al.* (1997).

PRODUCT TYPE & EMISSIONS						
PRODUCT TYPE (code)	SHORT DESCRIPTION	EMISSIONS EXPECTED TO*,**				
		STP	SURFACE WATER	SEDI-MENT	SOIL	OUTDOOR AIR
8.1	Wood preservative (industrial)	EQ ¹	EQ ²	EQ ³	EQ ⁴	N ⁵

* for notes: see table on preliminary environmental risk assessment in Mensink (1999).

** Y = yes; N = no; EQ = equivocal.

RCRs INITIAL & REFINED RISK ASSESSMENT & HAZARD GROUP					
PRODUCT TYPE (code)	SHORT DESCRIPTION	RCR*			HAZARD GROUP
		INITIAL	LOWEST	HIGHEST	
8.1	Wood preservative (industrial)	N.D.**	0.01	1?	NON-HAZARDOUS APPLICATION/UNKNOWN ¹¹

* for further details see Appendix 3, p. 103.

** N.D. is not determined.

¹¹ Non-hazardous refers to the impregnation process itself; unknown refers to emissions from impregnated sheet-piles.

REFINED ENVIRONMENTAL RISK ASSESSMENT

Refined risk assessment shows that an impregnation facility is not hazardous to the aquatic environment — with respect to arsenic pentoxide — with an RCR of 0.01. This is particularly due to the sorptive behaviour of arsenic in STPs. A second indirect route to the STP may be via the leaching of impregnated wood that is stored for drying on the industrial site. However, this route cannot be modelled by USES 2.0¹². It is estimated that max. 10 mg As/m³ wood per year) may dissipate to the soil via this route (Quarles van Ufford, 1994, cited in van Dokkum *et al.*, 1998).

Refined risk assessment also shows that arsenic pentoxide is a “disputable” substance with respect to emissions from sheet piles in water. It shows that a flux of 0.48% of the impregnated amount may cause a PEC that exceeds the PNEC. However, there is currently no clear evidence for this flux, which may imply that the substance should be denominated hazardous until further notice. The chemistry of arsenic in the environment is complex. Arsenic pentoxide in aqueous solution may give arsenate, followed by various complex reactions, dependent *e.g.* on the redox conditions. Most arsenic is expected to sorb to sediment or suspended matter in view of the partition coefficients as estimated by Crommentuijn *et al.* (1997)¹³. For reasons of convenience all DT₅₀'s in water used for the exposure assessment — *i.e.* hydrolysis, photolysis and biodegradation — are assumed to be 30 days. However, as long as the flux is not known, calculations even with the proper sorption data cannot be made.

The Board for the Authorisation of Pesticides stated on 31-03-2000 that for KEMWOOD CCA-C — one of the products containing arsenic pentoxide — it has not been shown that its use has no unacceptable effects on the environment, and that therefore the WG/GA¹⁴ has to be changed as follows: KEMWOOD CCA-C is registered as a wood preservative only, when the impregnated or drenched wood is not being processed or used by private persons, and when the treated wood is not used in direct or indirect contact with soil (including its use for sheet piling).

¹² Only concentrations in the soil due to the leaching of stored, impregnated wood can be modelled by USES 2.0. However, then particular retention data are required, that are not yet available.

¹³ Crommentuijn T., Polder M.D. & van de Plassche E.J. (1997) Maximum Permissible Concentrations and Negligible Concentrations for metals, taking background concentrations into account. RIVM Report no. 601501001. Partition coefficients for arsenic between particulate matter and water, soil and water, sediment and water are c. 1.0×10^5 , 190, and 6.6×10^4 dm³/kg, respectively.

¹⁴ Legal regulation and usage instructions (in Dutch: WG/GA).

bromoacetic acid

molecular weight	vapour pressure	water solubility	log K _{ow}
(-)	(Pa)	(mg/litre)	(-)
139.0	58*	9.0×10 ⁶	0.41*

* EPIWIN estimate (vapour pressure at 25 °C; log K_{ow} is an experimental value).

AQUATIC ENVIRONMENTAL/ECOTOXICOLOGICAL ENDPOINTS							
DT ₅₀ (hydrolysis)	DT ₅₀ (photolysis in water)	DT ₅₀ (biodegradation in water)	EC ₅₀ (STP microbes)	EC ₅₀ (algae)	E(L)C ₅₀ (crustaceans)	LC ₅₀ (fish)	BCF (fish)
(days)	(days)	(days)	(mg/litre)	(mg/litre)	(mg/litre)	(mg/litre)	(-)
-	-	*	-	0.29**	-	-	-

*EPIWIN indicates a probability of rapid biodegradation of 0.06-0.7.

** NOEC (algae) is 0.1 mg/litre.

PRODUCT TYPE & EMISSIONS						
PRODUCT TYPE (code)	SHORT DESCRIPTION	EMISSIONS EXPECTED TO*,**				
		STP	SURFACE WATER	SEDI-MENT	SOIL	OUTDOOR AIR
4	Food and feed area	EQ ¹	EQ ¹	EQ ¹	EQ ¹	EQ ¹

* for notes: see table on preliminary environmental risk assessment in Mensink (1999).

** Y = yes; N = no; EQ = equivocal.

RCRs INITIAL & REFINED RISK ASSESSMENT & HAZARD GROUP					
PRODUCT TYPE (code)	SHORT DESCRIPTION	RCR			HAZARD GROUP
		INITIAL	LOWEST	HIGHEST	
4	Food and feed area	N.D.*	N.D.	N.D.	UNKNOWN

* N.D. is not determined.

REFINED ENVIRONMENTAL RISK ASSESSMENT
No initial or refined risk assessment can be performed for the use of bromoacetic acid in the food and feed area. Ecotoxicity data for the effect analysis are lacking except an NOEC and an EC ₅₀ for algae. Besides, there is not a proper model for processing facilities in the food and feed area. The two products SEPTACID S and SEPTACID S PS are used for disinfecting the inner elements of process equipment in beer breweries. Therefore, it can be expected that after

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REFINED ENVIRONMENTAL RISK ASSESSMENT

rinsing, bromoacetic acid and its reactants — as it is a reactive substance of which the bromine part may react with organic material in the process water or effluent — will be discharged into the sewage system. In this way bromoacetic acid may not differ from the reactive and corrosive organochlorines that are used to release free chlorine for disinfection, showing a complex dissipation pattern, of which not much is known (*e.g.* sodium dichloroisocyanurate in Consultative expert group detergents-environment, 1989). In this context it is also important to state that the actual use of bromoacetic acid in the Netherlands may be high: in 1992 the yearly use was estimated to be 27,000 kg (VNCI, 1993). However, the major part of this use rate will be used in other facilities than beer breweries only.

In summary, emission of bromoacetic acid to municipal STPs cannot be excluded, though it seems unlikely in view of its reactivity. Therefore emission of the parent compound to fresh surface water via STP effluent may not occur. This may be different, however, for brominated reactants, as bromine is known to react with various organic molecules. There is not much known about these compounds and their environmental impact. Besides, there is no exposure model for food processing facilities, and there are no empirical data for confirmation (*e.g.* from monitoring).

cupric carbonate hydroxide

Syn.: cupric carbonate; copper (II) carbonate--copper (II) hydroxide (1:1)

molecular weight	vapour pressure	water solubility	log K _{ow}
(-)	(Pa)	(mg/litre)	(-)
221.1	-	1.0×10 ⁶ *	-

* EPIWIN estimate.

AQUATIC ENVIRONMENTAL/ECOTOXICOLOGICAL ENDPOINTS							
DT ₅₀ (hydrolysis)	DT ₅₀ (photolysis in water)	DT ₅₀ (biodegradation in water)	EC ₅₀ (STP microbes)	EC ₅₀ (algae)	E(L)C ₅₀ (crustaceans)	LC ₅₀ (fish)	BCF (fish)
(days)	(days)	(days)	(mg/litre)	(mg/litre)	(mg/litre)	(mg/litre)	(-)
-	-	-	-	*	*	*	-

* the MPA for aquatic organisms is 1.1 µg Cu/litre (Crommentuijn *et al.*, 1997).

PRODUCT TYPE & EMISSIONS						
PRODUCT TYPE	SHORT DESCRIPTION	EMISSIONS EXPECTED TO*,**				
(code)		STP	SURFACE WATER	SEDI-MENT	SOIL	OUTDOOR AIR
8.1	Wood preservative (industrial)	EQ ¹	EQ ²	EQ ³	EQ ⁴	N ⁵

* for notes: see table on preliminary environmental risk assessment in Mensink (1999).

** Y = yes; N = no; EQ = equivocal.

RCRs INITIAL & REFINED RISK ASSESSMENT & HAZARD GROUP					
PRODUCT TYPE	SHORT DESCRIPTION	RCR*			HAZARD GROUP
(code)		INITIAL	LOWEST	HIGHEST	
8.1	Wood preservative (industrial)	0.30	0.15	1?	NON-HAZARDOUS APPLICATION/UNKNOWN?

* for further details see Appendix 3, p. 108.

REFINED ENVIRONMENTAL RISK ASSESSMENT
Refined risk assessment shows that an impregnation facility is not hazardous to the aquatic environment — with respect to cupric carbonate hydroxide — with an RCR of 0.15. This is particularly due to the sorptive behaviour of copper in STPs. A second indirect route to the

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REFINED ENVIRONMENTAL RISK ASSESSMENT

STP may be via the leaching of impregnated wood that is stored for drying on the industrial site. However, this route cannot be modelled by USES 2.0¹⁵. Quarles van Ufford (1994, cited in van Dokkum *et al.*, 1998) estimated that copper impregnation with the vacuum-pressure method gave no copper residues in the process water, and that in 1990, leaching during storage could comprise as much as 130 mg copper per m³ wood. It is not clear what emissions of copper in the waste water may be caused by this leaching.

The Maximum Permissible Addition has been used as the PNEC. This MPA is the Maximum Permissible Concentration minus the background level (Crommentuijn *et al.*, 1997).

Refined risk assessment also shows that cupric carbonate hydroxide is a “disputable” substance with respect to emissions from sheet piles in water. It shows that a flux of 0.027% of the impregnated amount may cause a PEC that exceeds the PNEC. However, there is currently no clear evidence for this flux, which may imply that the substance should be denominated hazardous until further notice. Most copper is expected to sorb to sediment or suspended matter in view of the partition coefficients as estimated by Crommentuijn *et al.* (1997)¹⁶. However, as long as the flux is not known, calculations even with the proper sorption data cannot be made.

¹⁵ Only concentrations in the soil due to the leaching of stored, impregnated wood can be modelled by USES 2.0. However, then particular retention data are required, that are not yet available.

¹⁶ Crommentuijn T., Polder M.D. & van de Plassche E.J. (1997) Maximum Permissible Concentrations and Negligible Concentrations for metals, taking background concentrations into account. RIVM Report no. 601501001. Partition coefficients for copper between particulate matter and water, sediment and water are c. 5.0×10^4 and 3.4×10^4 dm³/kg, respectively.

disodium cyanodithioimido carbonate

Syn.: DNDIC

molecular weight	vapour pressure	water solubility	log K _{ow}
(-)	(Pa)	(mg/litre)	(-)
162.2	1.4*	2700*	0.31*

* EPIWIN estimate (vapour pressure and water solubility at 25 °C).

They refer to the non-salt. Actually the CAS no. also refers to the non-salt.

AQUATIC ENVIRONMENTAL/ECOTOXICOLOGICAL ENDPOINTS							
DT ₅₀ (hydrolysis)	DT ₅₀ (photolysis in water)	DT ₅₀ (biodegradation in water)	EC ₅₀ (STP microbes)	EC ₅₀ (algae)	E(L)C ₅₀ (crustaceans)	LC ₅₀ (fish)	BCF (fish)
(days)	(days)	(days)	(mg/litre)	(mg/litre)	(mg/litre)	(mg/litre)	(-)
0.29		60*	-	-	0.16-8.3**	74-120**	-

* EPIWIN indicates a probability of rapid biodegradation of 0.7-0.8. However, in view of lack of data, assumed to be 60 d for calculations (worst-case).

** EPA (1994).

PRODUCT TYPE & EMISSIONS						
PRODUCT TYPE	SHORT DESCRIPTION	EMISSIONS EXPECTED TO*,**				
(code)		STP	SURFACE WATER	SEDI-MENT	SOIL	OUTDOOR AIR
12.3	Slimicide (other)	EQ ¹	EQ ¹	EQ ¹	EQ ¹	EQ ¹

* for notes: see table on preliminary environmental risk assessment in Mensink (1999).

** Y = yes; N = no; EQ = equivocal.

RCRs INITIAL & REFINED RISK ASSESSMENT & HAZARD GROUP					
PRODUCT TYPE	SHORT DESCRIPTION	RCR*			HAZARD GROUP
(code)		INITIAL	LOWEST	HIGHEST	
12.3	Slimicide (other)	N.D.**	18	34375	VERY HAZARDOUS APPLICATION

* for further details see Appendix 3, p. 94.

** N.D. is not determined.

REFINED ENVIRONMENTAL RISK ASSESSMENT

Emission to outdoor air may occur, as disodium cyanodithioimido carbonate is volatile in view of its vapour pressure, and moderately volatile from water (dimensionless Henry's law constant is 2.5×10^{-5}). However, emission to outdoor air depends on the closeness of the process systems. Also monitoring data in air are not available. The calculations with USES 2.0 are a.o. based on physicochemical data generated by EPIWIN and referring to the non-salt.

Refined risk assessment shows that disodium cyanodithioimido carbonate is a very hazardous substance, when used as a slimicide. All scenarios indicate that the PECs exceed the PNEC. However, most scenarios are paper mill scenarios, whereas of course such equivalence between paper and sugar mills may be doubted. On the other hand, the EPA (1994) put paper and sugar mills together, with respect to occupational and residential exposure, and except for the EPA estimates there are no models available for estimating the emissions from sugar mills. Assuming that the Finnish approach is more realistic — due to the use of process temperature dependent hydrolysis and degradation rates — the PNEC is still exceeded largely under these more realistic assumptions. The USES 2.0 calculation with a worst-case assumption of 40 mg/litre process water does not seem to be unrealistic — when compared with the highest EPA estimate. However, it apparently refers to an atypical situation that may occur only once per — let's say — ten years.

It should be noted that disodium cyanodithioimido carbonate is very hazardous to aquatic organisms in spite of its very rapid hydrolysing. Probably a major part of the intoxication of aquatic organisms is due to (a) metabolite(s) of disodium cyanodithioimido carbonate. For all calculations, except those of the EPA for which the input data were not available, a $DT_{50, \text{hydrol, pH7, 25}^\circ\text{C}}$ of 7 hours is assumed. Hydrolysis is the major route of dissipation (EPA, 1994). At pH 5 and 7 thiocyanate (SCN^-) appears to be the major metabolite. At pH 9 other major metabolites — 3-amino-1,2,4-dithiazole-5-thione (thione) and 3-amino-1,2,4-dithiazole-5-oxone (oxone) — may be present as well. However, there are no monitoring data available on the occurrence of disodium cyanodithioimido carbonate or one of its hydrolytic products in the process water *c.q.* effluent.

glutaric aldehyde

Syn.: glutaral; glutaraldehyde; pentanedial

molecular weight	vapour pressure	water solubility	log K _{ow}
(-)	(Pa)	(mg/litre)	(-)
101.1	2.3×10 ³ *	1000**	-0.18***

* at 20 °C.

** actually readily soluble.

*** EPIWIN estimate.

AQUATIC ENVIRONMENTAL/ECOTOXICOLOGICAL ENDPOINTS							
DT ₅₀ (hydrolysis)	DT ₅₀ (photolysis in water)	DT ₅₀ (biodegradation in water)	EC ₅₀ (STP microbes)	EC ₅₀ (algae)	E(L)C ₅₀ (crustaceans)	LC ₅₀ (fish)	BCF (fish)
(days)	(days)	(days)	(mg/litre)	(mg/litre)	(mg/litre)	(mg/litre)	(-)
46*-102**	196*****	0.44******	17-25*	0.85*	0.55-465******	11-32*	-

* KEMI data (Eriksson *et al.*, 1995).

** at pH 7.0.

*** at pH 5.0.

**** EPIWIN indicates a probability of rapid biodegradation of 1.0.

***** a 21-d NOEC for *Daphnia magna* is 2.1 mg a.i./litre.

PRODUCT TYPE & EMISSIONS						
PRODUCT TYPE	SHORT DESCRIPTION	EMISSIONS EXPECTED TO*,**				
(code)		STP	SURFACE WATER	SEDI-MENT	SOIL	OUTDOOR AIR
2.1	Medical equipment	EQ ¹	EQ ²	EQ ³	EQ ⁴	N ⁵
2.4	Public health area (accommodation for man)	EQ ¹	EQ ²	EQ ³	EQ ⁴	N ⁵
2.10	Public health area (other)	EQ ¹	EQ ²	EQ ³	EQ ⁴	N ⁵
4	Food and feed area	EQ ¹	EQ ²	EQ ³	EQ ⁴	N ⁵
11	Liquid-cooling system preservative	N ¹	EQ ²	EQ ³	EQ ⁴	N ⁵
12.1	Slimeicide (paper industry)	Y ¹	Y ²	EQ ³	EQ ⁴	N ⁵

* for notes: see table on preliminary environmental risk assessment in Mensink (1999).

** Y = yes; N = no; EQ = equivocal.

*** the use for disinfecting veterinary medical equipment.

RCRs INITIAL & REFINED RISK ASSESSMENT & HAZARD GROUP					
PRODUCT TYPE	SHORT DESCRIPTION	RCR*			HAZARD GROUP
(code)		INITIAL	LOWEST	HIGHEST	
2.1	Public health area (med equipment)	N.D.**	0.07	8.0	“DISPUTABLY” HAZARDOUS APPLICATION
2.4	Public health area (accommodation for man)	0.06	0.1	0.1	NON-HAZARDOUS APPLICATION
2.10	Public health area (other)	N.D.	0.00009	0.03	NON-HAZARDOUS APPLICATION
4	Food and feed area	N.D.	N.D.	N.D.	UNKNOWN
11	Liquid-cooling system preservative	8,0	1619	1619	VERY HAZARDOUS APPLICATION
12.1	Slimicide (paper industry)	190	0.1	1333	VERY HAZARDOUS APPLICATION

* for further details see Appendix 3, p.95, 98 & 112.

** N.D. is not determined.

REFINED ENVIRONMENTAL RISK ASSESSMENT
<p>Refined risk assessment shows that the hazardousness of glutaric aldehyde is dependent on the type of use. It does not hydrolyse at room temperature — which may be the reason for its relative persistence in <i>e.g.</i> cooling-water systems — but it is assumed to be readily biodegradable in an STP. A major metabolite may be 3-formyl-6-hydroxy-2-cyclohexene-1-propanal which is a cyclic dimer of glutaric aldehyde (Eriksson <i>et al.</i>, 1995).</p> <p>Refined risk assessment shows that as a liquid-cooling system preservative the RCRs are high compared with the initial risk assessment (actually only a PEC assuming no hydrolysis or degradation could be calculated then) — in spite of introducing more realistic data on degradation. This may imply that for water-cooling biocides the “default” assumptions of the initial risk assessment rather refer to typical than to atypical conditions. This appears to be confirmed by some site-specific calculations measurements of glutaric aldehyde in the blow-down of some Dutch plants: Baltus <i>et al.</i> (1999) estimated PECs in the blow-down of cooling-water installations of 7500-44,000 µg/litre, which would give RCRs of 357-2095, a range that includes the calculated PEC for the refined risk assessment. These calculations, however, refer to plants that discharge their blow-off onto STPs. Therefore the final amounts of glutaric aldehyde in the recipient surface water — and thus the corresponding RCRs — are expected to be lower. The inclusion of a dilution factor of 3 for the recipient water — as a default for cooling-water installations in USES 2.0 — would lower the RCRs based on the data of Baltus <i>et al.</i> to 120-698. The hazardousness of glutaric aldehyde for the aquatic environment was also reported by Baltus <i>et al.</i> They stated that in toxicity tests glutaric aldehyde containing effluent of 2 facilities was acutely toxic to algae, crustaceans and fish.</p> <p>3-formyl-6-hydroxy-2-cyclohexene-1-propanal — a cyclic dimer of glutaric aldehyde — is assumed to be a major hydrolytic metabolite (Eriksson <i>et al.</i>, 1995).</p> <p>When used as a slimicide, the RCRs of the initial assessment are lower than those of the refined assessment: the adjusted USES scenario and two Finnish scenarios — one for an atypical paper mill with a very high waste water volume and one for a more typical plant, but with a worst-case concentration in process water — still exceed a PEC/PNEC of 1. The other Finnish and Swedish scenarios indicate that the substance is not hazardous. There is no clear explanation for these differences. However, the Finnish model — showing RCRs of 0.29-133, when assuming an additional dilution factor of 10 for the STP effluent to the recipient surface water — may be more realistic as it includes process temperature dependent hydrolysis and degradation. This appears to indicate that only under extreme conditions — very large plants, very high dosages — hazards may be expected.</p>

REFINED ENVIRONMENTAL RISK ASSESSMENT

In a Canadian paper mill with a paper production of 50-60 tonnes/day the concentration of glutaric aldehyde in the white water decreased rapidly from 51000 µg/litre half an hour after dosing to 4000 µg/litre, 6 hours after dosing, partly due to dilution of the white water (Eriksson *et al.*, 1995). In the white water effluent to the clarifier the concentration was already below the detection limit of 1000 µg/litre. Therefore PECs as reported above are difficult to verify, although the estimates of Eriksson *et al.* (1995) appear to be more likely than those of USES and the Finnish model mill 1.

Refined risk assessment for the use of glutaric aldehyde as a disinfectant in the public health area shows that glutaric aldehyde is probably not hazardous to the aquatic environment, except perhaps when used for disinfecting scopes with an RCR of 8.0. However, for this estimate it is assumed that all glutaric aldehyde in the Netherlands — 7000 kg in 1992 (VNCI, 1993) — is used for this purpose, which actually seems unlikely. Therefore, it can be expected that also for this purpose the actual RCR is ≤ 1 .

No initial or refined risk assessment can be performed for the use of glutaric aldehyde in the food and feed area as there is not a proper model for processing facilities in this area.

21

CAS no. 7789-29-9

potassium bifluoride

molecular weight	vapour pressure	water solubility	log K _{ow}
(-)	(Pa)	(mg/litre)	(-)
78.1	-	392,000	-

AQUATIC ENVIRONMENTAL/ECOTOXICOLOGICAL ENDPOINTS							
DT ₅₀ (hydrolysis)	DT ₅₀ (photolysis in water)	DT ₅₀ (biodegradation in water)	EC ₅₀ (STP microbes)	EC ₅₀ (algae)	E(L)C ₅₀ (crustaceans)	LC ₅₀ (fish)	BCF (fish)
(days)	(days)	(days)	(mg/litre)	(mg/litre)	(mg/litre)	(mg/litre)	(-)
-	-	-	-	-	-	-	-

PRODUCT TYPE & EMISSIONS						
PRODUCT TYPE	SHORT DESCRIPTION	EMISSIONS EXPECTED TO*,**				
(code)		STP	SURFACE WATER	SEDI-MENT	SOIL	OUTDOOR AIR
8.1	Wood preservative (industrial)	EQ ¹	EQ ²	N ³	N ⁴	N ⁵
8.2	Wood preservative (craft)	EQ ¹	EQ ²	N ³	N ⁴	N ⁵

* for notes: see table on preliminary environmental risk assessment in Mensink (1999).

** Y = yes; N = no; EQ = equivocal.

RCRs INITIAL & REFINED RISK ASSESSMENT & HAZARD GROUP					
PRODUCT TYPE	SHORT DESCRIPTION	RCR			HAZARD GROUP
(code)		INITIAL	LOWEST	HIGHEST	
8.1	Wood preservative (industrial)	N.D.*	N.D.	N.D.	NON-HAZARDOUS APPLICATION

*N.D. is not determined.

REFINED ENVIRONMENTAL RISK ASSESSMENT
<p>The registration of the IMPROSOL for dipping front carpentry in a special installation has expired since 01-03-2000. The WOODPIL product is processed into three types of plugs. This processing is entirely dry, there is no liquid effluent (person. communic. WOODCAP BV to RIVM). Potassium bifluoride should be considered as a non-hazardous substance with respect to the production process of the plugs.</p>

potassium hydroxide

molecular weight	vapour pressure	water solubility	log K _{ow}
(-)	(Pa)	(mg/litre)	(-)
56.1	-	1.1 × 10 ⁶ *	-

Source: NIA/VNCI (1998)¹⁷.

AQUATIC ENVIRONMENTAL/ECOTOXICOLOGICAL ENDPOINTS							
DT ₅₀ (hydrolysis)	DT ₅₀ (photolysis in water)	DT ₅₀ (biodegradation in water)	EC ₅₀ (STP microbes)	EC ₅₀ (algae)	E(L)C ₅₀ (crustaceans)	LC ₅₀ (fish)	BCF (fish)
(days)	(days)	(days)	(mg/litre)	(mg/litre)	(mg/litre)	(mg/litre)	(-)
-	-	-	-	-	-	80*	-

* the lowest LC₅₀ in IUCLID (1995).

PRODUCT TYPE & EMISSIONS						
PRODUCT TYPE	SHORT DESCRIPTION	EMISSIONS EXPECTED TO*,**				
(code)		STP	SURFACE WATER	SEDI-MENT	SOIL	OUTDOOR AIR
2.1	Public health area (medical equipment)	EQ ¹	EQ ²	N ³	N ³	N ³
4	Food and feed area	EQ ¹	EQ ²	N ³	N ³	N ³

* for notes: see table on preliminary environmental risk assessment in Mensink (1999).

** Y = yes; N = no; EQ = equivocal.

RCRs INITIAL & REFINED RISK ASSESSMENT & HAZARD GROUP					
PRODUCT TYPE	SHORT DESCRIPTION	RCR*			HAZARD GROUP
(code)		INITIAL	LOWEST	HIGHEST	
2.1	Medical equipment	N.D.**	0,0008	<2088	NON-HAZARDOUS APPLICATION
4	Food and feed area	N.D.	N.D.	N.D.	N.D.

* for further details see Appendix 3, p. 100.

** N.D. is not determined.

¹⁷ NIA/VNCI (1998) Chemiekaarten. Gegevens voor veilig werken met chemicaliën. 13e editie. Samson HD Tjeenk Willink, Alphen aan de Rijn.

REFINED ENVIRONMENTAL RISK ASSESSMENT

Refined risk assessment shows that the assumption of using all potassium hydroxide — that was used in 1992: *i.e.* 335.000 tonnes — for the disinfection of medical instruments other than endoscopes gives an RCR of 2088. In view of this assumption this RCR is very likely to be too high. The same calculation but with a default use of 250 kg/year — in conformity with van der Poel (1999) — gives a much lower RCR of 0.0008. Therefore it seems more plausible to designate potassium hydroxide as non-hazardous to the aquatic environment when used in the public health area. This fits with the notion that in an aqueous environment potassium hydroxide is a strong base and reacts violently with acids.

No initial or refined risk assessment can be performed for the use of potassium hydroxide in the food and feed area as there is not a proper model for processing facilities in this area. STPs may be expected to be loaded on a regular basis with biocides from a food or feed processing plant, but the exposure is not continuous (van Dokkum *et al.*, 1998). According to Van Dokkum *et al.*, however, potassium hydroxide is not one of the main biocides in the food and feed area. Therefore it remains to be seen, whether the use rate of potassium hydroxide in the food and feed area is high enough to cause a K^+ flux that substantially contributes to eutrophication of the effluent receiving surface water. Ecotoxicological effects, however, are not expected.

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CAS no. 137-41-7

potassium N-methyldithiocarbamate

Syn.: PNMDC

molecular weight	vapour pressure	water solubility	log K _{ow}
(-)	(Pa)	(mg/litre)	(-)
145.3	130*	4.4×10 ⁵ *	0.48*

* EPIWIN estimates (at 25 °C); they refer to the non-salt.

Actually the CAS no. also refers to the non-salt.

AQUATIC ENVIRONMENTAL/ECOTOXICOLOGICAL ENDPOINTS							
DT ₅₀ (hydrolysis)	DT ₅₀ (photolysis in water)	DT ₅₀ (biodegradation in water)	EC ₅₀ (STP microbes)	EC ₅₀ (algae)	E(L)C ₅₀ (crustaceans)	LC ₅₀ (fish)	BCF (fish)
(days)	(days)	(days)	(mg/litre)	(mg/litre)	(mg/litre)	(mg/litre)	(-)
*	*	*	-	-	0.028**	0.03-0.32**	-

* EPIWIN indicates a probability of rapid biodegradation of 0.7-0.8. As no data on persistence in water were available the DT₅₀'s used for calculations were assumed to be 30, 30 and 60 days for hydrolysis, photolysis and biodegradation, respectively (worst-case).

** refers to the a.i. of the 25% product BUSAN 881. This product also contains 20% disodium cyanodithioimido carbonate (see product profile).

PRODUCT TYPE & EMISSIONS						
PRODUCT TYPE	SHORT DESCRIPTION	EMISSIONS EXPECTED TO*,**				
(code)		STP	SURFACE WATER	SEDI-MENT	SOIL	OUTDOOR AIR
12.3	Slimicide (other)	EQ ¹	EQ ¹	EQ ¹	EQ ¹	EQ ¹

* for notes: see table on preliminary environmental risk assessment in Mensink (1999).

** Y = yes; N = no; EQ = equivocal.

RCRs INITIAL & REFINED RISK ASSESSMENT & HAZARD GROUP					
PRODUCT TYPE	SHORT DESCRIPTION	RCR*			HAZARD GROUP
(code)		INITIAL	LOWEST	HIGHEST	
12.3	Slimicide (other)	51,333	24,667	9,200,000	VERY HAZARDOUS APPLICATION

* for further details see Appendix 3, p. 96.

REFINED ENVIRONMENTAL RISK ASSESSMENT

Emission to outdoor air may occur, as potassium N-methyldithiocarbamate is volatile in view of its vapour pressure, and moderately volatile from water (dimensionless Henry's law constant is 1.7×10^{-5}), although this depends on the closeness of the process system. Monitoring data in air are not available. The calculations with USES 2.0 are a.o. based on physicochemical data generated by EPIWIN and referring to the non-salt.

Refined risk assessment shows that potassium N-methyldithiocarbamate is a very hazardous substance, when used as a slimicide. The scenarios indicate that the PECs always exceed the PNEC. However, the scenarios are paper mill scenarios, whereas of course such equivalence between paper and sugar mills may be doubted. Assuming that the Finnish approach is more "realistic" — due to the use of process temperature dependent hydrolysis and degradation rates — the PNEC is still exceeded largely under these more realistic assumptions. The USES 2.0 calculation with a worst-case assumption of 40 mg/litre process water gives an RCR of 51,300. As there are no other models or monitoring data available for verification, it remains difficult to determine the sense of realism of these initial and refined assessments. The lack of proper degradation data also hamper these assessments.

sodium dichloroisocyanurate

Syn.: troclosene sodium; 1,3,5-triazine-2,4,6(1H,3H,5H)-trione, 1,3-dichloro, sodium salt

molecular weight	vapour pressure	water solubility	log K _{ow}
(-)	(Pa)	(mg/litre)	(-)
220.0	1.9×10 ⁻¹² *	38,400*	-0.06*

* EPIWIN estimates (vapour pressure and water solubility at 25 °C).

AQUATIC ENVIRONMENTAL/ECOTOXICOLOGICAL ENDPOINTS							
DT ₅₀ (hydrolysis)	DT ₅₀ (photolysis in water)	DT ₅₀ (biodegradation in water)	EC ₅₀ (STP microbes)	EC ₅₀ (algae)	E(L)C ₅₀ (crustaceans)	LC ₅₀ (fish)	BCF (fish)
(days)	(days)	(days)	(mg/litre)	(mg/litre)	(mg/litre)	(mg/litre)	(-)
1->30*	-	**	-	-	0.18***	0.13***	-

* Surprisingly, the IUCLID data base reports a DT_{50,hydrol} of >30 days. However, in view of its reactivity, calculations have been performed with a DT₅₀ of 1 day.

** EPIWIN indicates a probability of rapid biodegradation of 0.5-0.6.

*** IUCLID (1995) data.

PRODUCT TYPE & EMISSIONS						
PRODUCT TYPE (code)	SHORT DESCRIPTION	EMISSIONS EXPECTED TO*,**				
		STP	SURFACE WATER	SEDI-MENT	SOIL	OUTDOOR AIR
2.2	Public health area (swimming pool)	EQ ¹	EQ ²	EQ ³	EQ ⁴	EQ ⁵
2.4	Public health area (accommodation for man)	N ¹	N ²	N ³	N ⁴	N ⁵
2.10	Public health area (other)	EQ ¹	EQ ²	EQ ³	EQ ⁴	N ⁵
4	Food and feed area	EQ ¹	EQ ²	EQ ³	EQ ⁴	N ⁵

* for notes: see table on preliminary environmental risk assessment in Mensink (1999).

** Y = yes; N = no; EQ = equivocal.

RCRs INITIAL & REFINED RISK ASSESSMENT & HAZARD GROUP					
PRODUCT TYPE	SHORT DESCRIPTION	RCR*			HAZARD GROUP
(code)		INITIAL	LOWEST	HIGHEST	
2.2	Swimming pool	N.D.**	20308	20308	VERY HAZARDOUS APPLICATION
2.4	Public health area (accommodation for man)	N.D.	71	71	VERY HAZARDOUS APPLICATION
2.10	Public health area (other)	N.D.	10	3077	VERY HAZARDOUS APPLICATION
4	Food and feed area	N.D.	N.D.	N.D.	N.D.

* for further details see Appendix 3, p. 101.

** N.D. is not determined.

REFINED ENVIRONMENTAL RISK ASSESSMENT
<p>Refined risk assessment shows that the use of sodium dichloroisocyanurate appears to be very hazardous independent of the type of use. However, this may be due to the inappropriateness of USES to deal with such a very rapidly hydrolysing biocide (see below). It should be noted that sodium dichloroisocyanurate hydrolyses rapidly and therefore will not reach the STP as such. Major metabolites are hypochlorous acid and cyanuric acid. In fresh water hypochlorous acid is assumed to dissipate within 15 minutes (RIVM, 1998), probably mainly by forming OCl⁻ and H⁺, of which the first can be remarkably stable in aqueous solutions. Therefore exposure to this metabolite — that is very toxic to aquatic organisms (RIVM, 1998) — under particular conditions may occur (unless it can be shown that it will not pass the STP). The PNEC is based on the ecotoxicity data of the IUCLID database. As these data are only briefly reported, no appropriate exposure analysis is possible. It is therefore not clear whether the effects are due to the parent compound, hypochlorous acid, cyanuric acid or some other residue. However, chlorinated isocyanurates are very highly toxic to coldwater fish, highly toxic to freshwater fish, highly toxic to freshwater invertebrates and very highly toxic to estuarine and marine organisms (EPA, 1992b). Therefore the concentrations < 500 µg cyanuric/litre in STPs — that emission experts assume to be low (see Consultative expert group detergents-environment, 1989) — may still be detrimental to aquatic organisms. In conclusion, the outcomes with respect to sodium dichloroisocyanurate are tentative and will need further study.</p> <p>The refined risk assessment in the public health area 2.10 refer to the use of sodium dichloroisocyanurate in hospitals for disinfecting rooms, furniture and objects in hospitals (RCR of 538), in tumbler machines for washing hospital laundry (RCR of 10) and in washing streets for washing hospital laundry (RCR of 3077).</p> <p>No initial or refined risk assessment can be performed for the use of sodium dichloroisocyanurate in the food and feed area as there is not a proper model for processing facilities in this area.</p> <p>VNCI (1993) estimated the total use rate of sodium dichloroisocyanurate in 1992 in the Netherlands of c. 56,000 kg, but it is not clear which product type shows the highest use.</p>

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CAS no. 7681-52-9

sodium hypochlorite

Syn.: hypochlorous acid, sodium salt

molecular weight	vapour pressure	water solubility	log K _{ow}
(-)	(Pa)	(mg/litre)	(-)
74.4	-	1000*	-

* NaOCl is assumed to be ready water soluble.

AQUATIC ENVIRONMENTAL/ECOTOXICOLOGICAL ENDPOINTS							
DT ₅₀ (hydrolysis)	DT ₅₀ (photolysis in water)	DT ₅₀ (biodegradation in water)	EC ₅₀ (STP microbes)	EC ₅₀ (algae)	E(L)C ₅₀ (crustaceans)	LC ₅₀ (fish)	BCF (fish)
(days)	(days)	(days)	(mg/litre)	(mg/litre)	(mg/litre)	(mg/litre)	(-)
-	-	0.01	-	-	0.07-52-	0.02*-10	-

* the lowest LC₅₀ in IUCLID (1995).

PRODUCT TYPE & EMISSIONS						
PRODUCT TYPE	SHORT DESCRIPTION	EMISSIONS EXPECTED TO*,**				
(code)		STP	SURFACE WATER	SEDI-MENT	SOIL	OUTDOOR AIR
2.4	Public health area (accommodation for man)	N ¹	N ²	N ³	N ⁴	N ⁵
4	Food and feed area	EQ ¹	N ²	N ³	N ⁴	N ⁵
11	Liquid-cooling system preservative	N ¹	Y ²	N ³	N ⁴	N ⁵

* for notes: see table on preliminary environmental risk assessment in Mensink (1999).

** Y = yes; N = no; EQ = equivocal.

RCRs INITIAL & REFINED RISK ASSESSMENT & HAZARD GROUP*					
PRODUCT TYPE	SHORT DESCRIPTION	RCR*			HAZARD GROUP
(code)		INITIAL	LOWEST	HIGHEST	
2.4	Public health area (accommodation for man)	2000	600	600	VERY HAZARDOUS APPLICATION
2.10	Public health area (other)**	N.D.***	30	30	HAZARDOUS APPLICATION
4	Food and feed area	N.D.	N.D.	N.D.	UNKNOWN
11	Liquid-cooling system preservative	8500	333,500	333,500	VERY HAZARDOUS APPLICATION

* for further details see Appendix 3, p. 99 & 112.

** used for disinfecting rooms, furniture and objects in hospitals.

*** N.D. is not determined.

REFINED ENVIRONMENTAL RISK ASSESSMENT

Refined risk assessment shows that sodium hypochlorite is a hazardous or very hazardous substance. It should be noted that sodium hypochlorite is very reactive. Therefore no hypochlorite or free chlorine is expected to pass an STP. However, various chlorine containing microcontaminants can be formed varying from chloramines and chloroform to mono, di, and trichloroacetic acid (RIVM, 1998). The major metabolite appears to be hypochlorous acid, of which OCl^- can be remarkably stable in aqueous solutions. However, it is not expected to pass an STP, and therefore USES 2.0 is probably not suitable to deal with such very reactive substances (as in case of not passing an STP the PEC/PNEC ratio would be nil). This might be different for other metabolites. Due to chlorination of fresh water bromated microcontaminants can also be formed. Organic molecules as fulvic and humic acids may react with chlorine as well.

Sodium hypochlorite is rapidly degraded by activated sludge at a rate of 10.7 mg/litre with a DT_{50} of less than two minutes. Effects of sodium hypochlorite on the effectiveness of an STP are probably low (RIVM, 1998). Reported effects at daily dosages up to 125 mg/litre caused at most a slight reduction of the removal capacity, probably due to the free chlorine in the system. Continuous application of sodium hypochlorite, on the other hand, showed an EC_{50} for the respiration of active sludge of 3 mg/litre and an NOEC of 0.38 mg/litre. In view of its reactivity concentrations are expected to be far below this NOEC.

Refined risk assessment for the use of sodium hypochlorite as a disinfectant in the public health area shows that sodium hypochlorite is still (very) hazardous to the aquatic environment. As stated above the sense of realism of this statement may be doubted in view of the reactivity of sodium hypochlorite.

Refined risk assessment shows that as a liquid-cooling system preservative the RCRs are high compared with the initial risk assessment (actually only a PEC assuming no hydrolysis or degradation was calculated then) — in spite of introducing more realistic data on hydrolysis and degradation. This may imply that for cooling-water biocides the “default” assumptions of the initial risk assessment rather refer to typical than to atypical conditions. The hazardousness of sodium hypochlorite for the aquatic environment was also reported by Baltus *et al.* (1999). They stated that in toxicity tests sodium hypochlorite (or its metabolites) containing effluent of 3 facilities using this substance only was acutely toxic to algae.

No initial or refined risk assessment can be performed for the use of sodium hypochlorite in the food and feed area as there is not a proper model for processing facilities in this area.

sodium p-toluenesulfonchloramide

molecular weight	vapour pressure	water solubility	log K _{ow}
(-)	(Pa)	(mg/litre)	(-)
205.7	0.022*	1.5×10 ⁵ *	0.84*

* EPIWIN estimates (vapour pressure and water solubility at 25 °C).

AQUATIC ENVIRONMENTAL/ECOTOXICOLOGICAL ENDPOINTS							
DT ₅₀ (hydrolysis)	DT ₅₀ (photolysis in water)	DT ₅₀ (biodegradation in water)	EC ₅₀ (STP microbes)	EC ₅₀ (algae)	E(L)C ₅₀ (crustaceans)	LC ₅₀ (fish)	BCF (fish)
(days)	(days)	(days)	(mg/litre)	(mg/litre)	(mg/litre)	(mg/litre)	(-)
2	-	*	-	80	4.5**	31***	-

* EPIWIN indicates a probability of rapid biodegradation of 0.7.

** a 21-d NOEC for *Daphnia magna* was 1.1 a.i. mg/litre (IUCLID, 1995). The MATC for this 21-d test was calculated to be 2 mg a.i./litre.

*** a 35-d NOEC for *Pimephales promelas* was 1.5 mg a.i./litre (IUCLID, 1995).

PRODUCT TYPE & EMISSIONS						
PRODUCT TYPE	SHORT DESCRIPTION	EMISSIONS EXPECTED TO*,**				
(code)		STP	SURFACE WATER	SEDI-MENT	SOIL	OUTDOOR AIR
2.4	Public health area (accommodation for man)	EQ ¹	EQ ²	EQ ³	EQ ⁴	N ⁵
2.10	Public health area (other, <i>i.c.</i> laundry)	EQ ¹	EQ ²	EQ ³	EQ ⁴	N ⁵
4	Food and feed area	EQ ¹	EQ ²	EQ ³	EQ ⁴	N ⁵

* for notes: see table on preliminary environmental risk assessment in Mensink (1999).

** Y = yes; N = no; EQ = equivocal.

RCRs INITIAL & REFINED RISK ASSESSMENT & HAZARD GROUP					
PRODUCT TYPE	SHORT DESCRIPTION	RCR*			HAZARD GROUP
(code)		INITIAL	LOWEST	HIGHEST	
2.4	Public health area (accommodation for man)	0.77	0.05	5.0	“DISPUTABLY” HAZARDOUS APPLICATION
2.10	Public health area (other)	N.D.**	0.005	1.6	“DISPUTABLY” HAZARDOUS APPLICATION
4	Food and feed area	N.D.	N.D.	N.D.	UNKNOWN

* for further details see Appendix 3, p. 102.

** N.D. is not determined.

REFINED ENVIRONMENTAL RISK ASSESSMENT

Refined risk assessment shows that the use of sodium p-toluenesulfonchloramide appears to be “disputably” hazardous independent of the type of use. Sodium p-toluenesulfonchloramide hydrolyses readily to hypochlorite and para-toluenesulfonamide; hypochlorite forms free chlorine, that is assumed to be the disinfecting agent (see also sodium hypochlorite, biocide no. 25). The PNEC is based on the ecotoxicity data of the IUCLID database. As these data are only briefly reported, no appropriate exposure analysis is possible. It is *e.g.* not clear whether the effects are due to the parent compound, or (a) metabolite(s). For further conclusions the reader is kindly referred to sodium hypochlorite (biocide no. 25).

For the initial risk assessment no hydrolysis or degradation was assumed (as these data were not available then). The refined risk assessment in the public health area 2.10 refers to the use of sodium p-toluenesulfonchloramide in cleaning hospital rooms and furniture (RCR of 0.55), in tumbler machines for washing hospital laundry (RCR of 0.005) and in washing streets for hospital laundry (RCR of 1.6).

No initial or refined risk assessment can be performed for the use of sodium p-toluenesulfonchloramide in the food and feed area as there is not a proper model for processing facilities in this area.

Effects of sodium p-toluenesulfonchloramide on activated sludge are probably low as the respiration was inhibited at high concentrations of 124-250 mg/litre.

VNCI (1993) estimated the total use rate of sodium p-toluenesulfonchloramide in 1992 in the Netherlands of c. 6,900 kg, but it is not clear which product type shows the highest use.

27

CAS no. -

zinc borate

molecular weight	vapour pressure	water solubility	log K _{ow}
(-)	(Pa)	(mg/litre)	(-)
314.0	-	-	-

AQUATIC ENVIRONMENTAL/ECOTOXICOLOGICAL ENDPOINTS							
DT ₅₀ (hydrolysis)	DT ₅₀ (photolysis in water)	DT ₅₀ (biodegradation in water)	EC ₅₀ (STP microbes)	EC ₅₀ (algae)	E(L)C ₅₀ (crustaceans)	LC ₅₀ (fish)	BCF (fish)
(days)	(days)	(days)	(mg/litre)	(mg/litre)	(mg/litre)	(mg/litre)	(-)
-	-	-	-	-	-	-	-

PRODUCT TYPE & EMISSIONS						
PRODUCT TYPE (code)	SHORT DESCRIPTION	EMISSIONS EXPECTED TO*,**				
		STP	SURFACE WATER	SEDI-MENT	SOIL	OUTDOOR AIR
2.4	Public health area (accommodation for man)	EQ ¹	EQ ¹	EQ ¹	EQ ¹	EQ ¹
2.5	Public health area (industrial area)	EQ ¹	EQ ¹	EQ ¹	EQ ¹	EQ ¹
21	Antifouling product	EQ ¹	EQ ¹	EQ ¹	EQ ¹	EQ ¹

* for notes: see table on preliminary environmental risk assessment in Mensink (1999).

** Y = yes; N = no; EQ = equivocal.

REFINED ENVIRONMENTAL RISK ASSESSMENT
<p>No refined risk assessment was performed as zinc borate was not among the substance-specific applications with the highest abundance. Besides, the only registered product — ALBOFIX — has been withdrawn from the market since 01-01-2000. The final date until which the already stored cans can be sold is 01-01-2001.</p>

zinc oxalate

molecular weight	vapour pressure	water solubility	log K _{ow}
(-)	(Pa)	(mg/litre)	(-)
153.4	1.7×10 ⁻⁴ *	0.05**	-0.9*

* EPIWIN estimates (at 25°C).

** actually very slightly soluble.

AQUATIC ENVIRONMENTAL/ECOTOXICOLOGICAL ENDPOINTS							
DT ₅₀ (hydrolysis)	DT ₅₀ (photolysis in water)	DT ₅₀ (biodegradation in water)	EC ₅₀ (STP microbes)	EC ₅₀ (algae)	E(L)C ₅₀ (crustaceans)	LC ₅₀ (fish)	BCF (fish)
(days)	(days)	(days)	(mg/litre)	(mg/litre)	(mg/litre)	(mg/litre)	(-)
-	-	*	-	-	-	-	-

* EPIWIN indicates a probability of rapid biodegradation of 0.7.

PRODUCT TYPE & EMISSIONS						
PRODUCT TYPE (code)	SHORT DESCRIPTION	EMISSIONS EXPECTED TO*,**				
		STP	SURFACE WATER	SEDI-MENT	SOIL	OUTDOOR AIR
2.4	Public health area (accommodation for man)	EQ ¹	N ²	N ²	EQ ³	N ⁴
2.5	Public health area (industrial area)	EQ ¹	N ²	N ²	EQ ³	N ⁴
21	Antifouling product	N ¹	EQ ²	EQ ²	N ³	N ⁴

* for notes: see table on preliminary environmental risk assessment in Mensink (1999).

** Y = yes; N = no; EQ = equivocal.

REFINED ENVIRONMENTAL RISK ASSESSMENT
<p>No refined risk assessment was performed as zinc oxalate was not among the substance-specific applications with the highest abundance. Besides, the only registered product — ALBOFIX — has been withdrawn from the market since 01-01-2000. The final date until which the already stored cans can be sold is 01-01-2001.</p>

Appendix 2 EU biocidal product types (PT)

- PT 1: Human hygiene biocidal products.
Fields of use: 1.1 Skin antiseptic.
 1.2 Antimicrobial soap and health care personnel handwash.
 1.3 Others.
- PT 2: Private area and public health area disinfectants and other biocidal products.
Fields of use: 2.1 Medical equipment.
 2.2 Swimming pool, aquarium bathing and other waters.
 2.3 Air-conditioning system.
 2.4 Accommodation for man.
 2.5 Industrial areas.
 2.6 Chemical toilets.
 2.7 Waste water.
 2.8 Hospital waste.
 2.9 Soil or other substrates.
 2.8 Others (*e.g.* hospital laundry).
- PT 3: Veterinary hygiene biocidal products.
Fields of use: 3.1 Housing facilities, and transportation means.
 3.2 Milking machines.
 3.3 Applied directly to animals (udder cleaning, eggs before incubation).
 3.4 Others.
- PT 4: Food and feed area disinfectants.
- PT 5: Drinking water disinfectants.
- PT 6: In-can preservatives.
Fields of use: 6.1 Human hygiene products.
 6.2 Detergents.
 6.3 Others.
- PT 7: Film preservatives.
- PT 8: Wood preservatives.
Fields of use: 8.1 Pre-treatment in industrial premises.
 8.2 Professional non-industrial treatment, for example remedial application.
 8.3 General use surface protection.

PT 9: Fibre, leather, rubber, and polymerised materials preservatives.

- Fields of use:
- 9.1 Textile.
 - 9.2 Leather.
 - 9.3 Rubber and polymerised material.
 - 9.4 Paper.
 - 9.5 Others.

PT 10: Masonry preservatives.

PT 11: Preservatives for liquid-cooling and processing systems.

PT 12: Slimicides.

- Fields of use:
- 12.1 Paper industry.
 - 12.2 Oil extraction industry.
 - 12.3 Others (*e.g.* sugar industry).

PT 13: Metalworking-fluid preservatives.

PT 14: Rodenticides.

PT 15: Avicides.

PT 16: Molluscicides.

PT 17: Piscicides.

PT 18: Insecticides, acaricides and products to control other arthropods.

PT 19: Repellants and attractants.

- Fields of use:
- 19.1 Repellant applied to humans skin.
 - 19.2 Repellant applied to animals skin.
 - 19.3 Other repellants.
 - 19.4 Attractants.

PT 20: Preservatives for food and feedstocks.

PT 21: Antifouling products.

- Fields of use:
- 21.1 On boats and ships.
 - 21.2 Aquaculture equipment and other immersed structure.

PT 22: Embalming and taxidermist fluids.

PT 23: Control of other vertebrates.

Appendix 3 Risk characterisation spreadsheets per priority substance

The rows in grey refer to the initial aquatic environmental risk assessment as reported in Mensink (1999). The other rows refer to the refined risk assessment.

For reasons of convenience the reference Eriksson *et al.* (1995) has been abbreviated to KEMI (1995).

Slimicide: 2,2-dibromo-3-nitrilopropionamide

	PEC or PNEC	source	value	dimension	comments	PEC/PNEC
	PNEC	KEMI, 1995; Mensink, 1999	0,3	µg/litre	PNEC based on algae (EC ₅₀ /1000); calculation conform MPC-protocol (Kalf <i>et al.</i> , 1999)	
1	PEC _{surface water}	model USES (Mensink, 1999)	250	µg/litre	waste water volume 3000 m ³ /d; dilution factor in receiving water 10; worst-case input concentration process water (i.e. 40 mg/litre) ; DT _{50,hydroly} is 1,5 days; log K _{ow} assumed to be 7,7(probably erroneously reported in unpublished RIVM report); no biodegradation is assumed due to lack of data (Mensink, 1999); STP included	833
2	PEC _{surface water}	model USES	172	µg/litre	waste water volume 3000 m ³ /d; dilution factor in receiving water 10; more realistic input concentration process water (i.e. 5 mg/litre) ; DT _{50,hydroly} is 2,6 days (KEMI, 1995); log K _{ow} is 0,84 (KEMI, 1995); DT _{50,biodeg,wat/seq} is 0,21 days (KEMI, 1995); WWTP included: DT _{50,biodeg,STP} is arbitrarily assumed to be [DT _{50,biodeg,wat/seq}]/2; K_{oc} is 32 dm³/kg (KEMI, 1995)	573
3	PEC _{surface water}	model USES	162	µg/litre	waste water volume 3000 m ³ /d; dilution factor in receiving water 10; more realistic input concentration process water (i.e. 5 mg/litre) ; DT _{50,hydroly} is 2,6 days (KEMI, 1995); log K _{ow} is 0,84 (KEMI, 1995); DT _{50,biodeg,wat/seq} is 0,21 days (KEMI, 1995); WWTP included: DT _{50,biodeg,STP} is arbitrarily assumed to be [DT _{50,biodeg,wat/seq}]/2; K_{oc} is 663 dm³/kg (KEMI, 1995)	540
4	PEC _{surface water}	Finnish model mill 1	0,38	µg/litre	540 ton/d; waste water volume 800 m ³ /h (higher than normal); waste water temperature 55 °C; residence time of water 0,5 h prior to entrance WWTP with activated sludge; DT ₅₀ 's are corrected for process temperatures	1
5	PEC _{surface water}	Finnish model mill 2	0,018	µg/litre	lower waste water volume than mill 1: 8740 m ³ /d (of which 60% from the short circulation of the wire part); further as mill 1; worst-case input concentration process water worst-case (i.e. 40 mg/litre) ; DT ₅₀ 's are corrected for process temperatures	0,06
6	PEC _{surface water}	Finnish model mill 2	0,002	µg/litre	lower waste water volume than mill 1: 8740 m ³ /d (of which 60% from the short circulation of the wire part); further as mill 1; more realistic input concentration process water (i.e. 5 mg/litre) ; DT ₅₀ 's are corrected for process temperatures	0,01
7	PEC _{surface water}	KEMI scenario 1	3,9	µg/litre	fine paper mill; water consumption 5000 m ³ /d; 300 m ³ white water; two dosages per day; more realistic scenario (input concentration process water 5 mg/litre)	13
8	PEC _{surface water}	KEMI scenario 2	1,7	µg/litre	newspaper mill A (2 days retention time); water consumption 25000 m ³ /d; 1000 m ³ white water; two dosages per day; more realistic scenario (input concentration process water 5 mg/litre)	6
9	PEC _{surface water}	KEMI scenario 3	0,77	µg/litre	newspaper mill B; water consumption 28000 m ³ /d; 300 m ³ white water; two dosages per day; realistic scenario (input concentration process water 5 mg/litre)	3

The abovementioned application of 2,2-dibromo-3-nitrilopropionamide is very hazardous (2 of 8 refined scenarios)

Slimicide: 2-bromo-4-hydroxyacetofenone

PEC or PNEC	source	value	dimension	comments	PEC/PNEC	
PNEC	KEMI, 1995; Mensink, 1999	0,14	µg/litre	PNEC based on crustaceans (21-d NOEC/100); calculation conform MPC-protocol (Kalf <i>et al.</i> , 1999)		
1	PEC _{surface water}	model USES (Mensink, 1999)	4000	µg/litre	waste water volume 3000 m ³ /d; dilution factor in receiving water 10; worst-case input concentration process water (i.e. 40 mg/litre) ; STP included, though no biodegradation is assumed; DT _{50,hydroly} is 16 days; photolysis is assumed not to occur prior to effluent discharge (worst case); no sorption data available	28571
2	PEC _{surface water}	model USES	3480	µg/litre	waste water volume 3000 m ³ /d; dilution factor in receiving water 10; worst-case input concentration process water (i.e. 40 mg/litre) ; STP included; DT _{50,biodeg,STP} is 1,4 days; DT _{50,biodeg,wat/sed} is 2,8 days; DT _{50,hydroly} is 16 days; photolysis is assumed not to occur prior to effluent discharge (worst case); no sorption data available	24857
3	PEC _{surface water}	model USES	79	µg/litre	waste water volume 3000 m ³ /d; dilution factor in receiving water 10; more realistic input concentration process water (i.e. 0,9 mg/litre) ; STP included; no sorption data available (further assumptions as above)	564
4	PEC _{surface water}	Finnish model mill 1	1804	µg/litre	540 ton/d; waste water volume 800 m ³ /h (higher than normal); waste water temperature 55 °C; residence time of water 0,5 h prior to entrance STP with activated sludge	12886
5	PEC _{surface water}	Finnish model mill 2	100	µg/litre	lower waste water volume than mill 1: 8740 m ³ /d (of which 60% from the short circulation of the wire part); further as mill 1; worst-case input concentration process water worst-case (i.e. 40 mg/litre)	714
6	PEC _{surface water}	Finnish model mill 2	2	µg/litre	lower waste water volume than mill 1: 8740 m ³ /d (of which 60% from the short circulation of the wire part); further as mill 1; more realistic input concentration process water (i.e. 0,9 mg/litre)	14
7	PEC _{surface water}	KEMI scenario 1	0,98	µg/litre	fine paper mill; water consumption 5000 m ³ /d; 300 m ³ white water; two dosages per day; more realistic scenario (input concentration process water 0,9 mg/litre)	7
8	PEC _{surface water}	KEMI scenario 2	0,4	µg/litre	newspaper mill A (2 days retention time); water consumption 25000 m ³ /d; 1000 m ³ white water; two dosages per day; more realistic scenario (input concentration process water 0,9 mg/litre)	3
9	PEC _{surface water}	KEMI scenario 3	0,14	µg/litre	newspaper mill B; water consumption 28000 m ³ /d; 300 m ³ white water; two dosages per day; realistic scenario (input concentration process water 0,9 mg/litre)	1

The abovementioned application of 2-bromo-4-hydroxyacetofenone is very hazardous (4 of 8 refined scenarios)

Slimicide: 1,2-benzisothiazolin-3-one

	PEC or PNEC	source	value	dimension	comments	PEC/PNEC
	PNEC	KEMI, 1995; Mensink, 1999	1,1	µg/litre	PNEC based on crustaceans (EC ₅₀ /1000); calculation conform MPC-protocol (Kalf <i>et al.</i> , 1999)	
1	PEC _{surface water}	model USES (Mensink, 1999)	3990	µg/litre	waste water volume 3000 m ³ /d; dilution factor in receiving water 10; worst-case input concentration process water (i.e. 40 mg/litre) ; no hydrolysis or degradation is assumed (due to lack of data); STP included	3627
2	PEC _{surface water}	model USES	2860	µg/litre	waste water volume 3000 m ³ /d; dilution factor in receiving water 10; worst-case input concentration process water (i.e. 40 mg/litre) ; assuming data on the degradation of isothiazolines in general: DT _{50,hydrat,25 °C,pH 8} is 11 days and DT _{50,biodeg,wat/seq} is max. 1 day (Baltus & Berbee, 1996); STP included	2600
3	PEC _{surface water}	model USES	no data	µg/litre	waste water volume 3000 m ³ /d; dilution factor in receiving water 10; more realistic input concentration process water not available ; STP included	no data
4	PEC _{surface water}	Finnish model mill 1	3	µg/litre	540 ton/d; waste water volume 800 m ³ /h (higher than normal); waste water temperature 55 °C; residence time of water 0,5 h prior to entrance STP with activated sludge; DT ₅₀ 's corrected for process temperatures	2,7
5	PEC _{surface water}	Finnish model mill 2	2	µg/litre	lower waste water volume than mill 1: 8740 m ³ /d (of which 60% from the short circulation of the wire part); further as mill 1; worst-case input concentration process water worst-case (i.e. 40 mg/litre) ; DT ₅₀ 's corrected for process temperatures	1,8
6	PEC _{surface water}	Finnish model mill 2	no data	µg/litre	lower waste water volume than mill 1: 8740 m ³ /d (of which 60% from the short circulation of the wire part); further as mill 1; more realistic input concentration process water not available	no data
7	PEC _{surface water}	KEMI scenario 1	no data	µg/litre	fine paper mill; water consumption 5000 m ³ /d; 300 m ³ white water; two dosages per day; more realistic scenario (input concentration process water not available)	no data
8	PEC _{surface water}	KEMI scenario 2	no data	µg/litre	newspaper mill A (2 days retention time); water consumption 25000 m ³ /d; 1000 m ³ white water; two dosages per day; more realistic scenario (input concentration process water not available)	no data
9	PEC _{surface water}	KEMI scenario 3	no data	µg/litre	newspaper mill B; water consumption 28000 m ³ /d; 300 m ³ white water; two dosages per day; realistic scenario (input concentration process water not available)	no data

The abovementioned application of 1,2-benzisothiazolin-3-one is very hazardous (1 of 3 refined scenarios)

Slimicide: 2-methyl-4-isothiazolin-3-one

PEC or PNEC	source	value	dimension	comments	PEC/PNEC	
PNEC	KEMI, 1995; EPA, 1998; Mensink, 1999	0,7	µg/litre	PNEC based on the lowest of two chronic MATCs (crustaceans & fish) (MATC/50); calculation conform MPC-protocol (Kalf <i>et al.</i> , 1999)		
1	PEC _{surface water}	model USES (Mensink, 1999)	3960	µg/litre	waste water volume 3000 m ³ /d; dilution factor in receiving water 10; worst-case input concentration process water (i.e. 40 mg/litre) ; no sorption data (therefore the sorption is based on the log K _{ow}); no hydrolysis or biodegradation is assumed due to lack of data (Mensink, 1999)	5657
2	PEC _{surface water}	model USES	26	µg/litre	waste water volume 3000 m ³ /d; dilution factor in receiving water 10; more realistic input concentration process water (i.e. 0,55 mg/litre) ; DT _{50,biodeg, wat/seg} is 0,38 days at 25 °C (KEMI, 1995); DT _{50,biodeg, STP} is arbitrarily assumed to be [DT _{50,biodeg, wat/seg}]/2;	37
3	PEC _{surface water}	Finnish model mill 1	9	µg/litre	540 ton/d; waste water volume 800 m ³ /h (higher than normal); waste water temperature 55 °C; residence time of water 0,5 h prior to entrance STP with activated sludge; DT ₅₀ 's corrected for process temperatures	13
4	PEC _{surface water}	Finnish model mill 2	0,18	µg/litre	lower waste water volume than mill 1: 8740 m ³ /d (of which 60% from the short circulation of the wire part); further as mill 1; worst-case input concentration process water worst-case (i.e. 40 mg/litre) ; DT ₅₀ 's corrected for process temperatures	0,26
5	PEC _{surface water}	Finnish model mill 2	0,002	µg/litre	lower waste water volume than mill 1: 8740 m ³ /d (of which 60% from the short circulation of the wire part); further as mill 1; more realistic input concentration process water (i.e. 0,55 mg/litre) ; DT ₅₀ 's corrected for process temperatures	0,0029
6	PEC _{surface water}	KEMI scenario 1	0,66	µg/litre	fine paper mill; water consumption 5000 m ³ /d; 300 m ³ white water; two dosages per day; more realistic scenario (input concentration process water 0,55 mg/litre)	0,94
7	PEC _{surface water}	KEMI scenario 2	0,088	µg/litre	newspaper mill A (2 days retention time); water consumption 25000 m ³ /d; 1000 m ³ white water; two dosages per day; more realistic scenario (input concentration process water 0,55 mg/litre)	0,13
8	PEC _{surface water}	KEMI scenario 3	0,046	µg/litre	newspaper mill B; water consumption 28000 m ³ /d; 300 m ³ white water; two dosages per day; realistic scenario (input concentration process water 0,55 mg/litre)	0,07

The abovementioned application of 2-methyl-4-isothiazolin-3-one is hazardous (2 of 7 refined scenarios)

Slimicide: 5-chloro-2-methyl-4-isothiazolin-3-one

PEC or PNEC	source	value	dimension	comments	PEC/PNEC	
PNEC	KEMI, 1995; EPA, 1998; Mensink, 1999	2	µg/litre	PNEC based on 2 additional NOECs for the different taxonomic groups: 0,10/50; calculation conform MPC-protocol (Kalf <i>et al.</i> , 1999)		
1	PEC _{surface water}	model USES (Mensink, 1999)	4000	µg/litre	waste water volume 3000 m ³ /d; dilution factor in receiving water 10; worst-case input concentration process water (i.e. 40 mg/litre) ; no hydrolysis or biodegradation was assumed due to lack of data (Mensink, 1999)	2000
2	PEC _{surface water}	model USES	50	µg/litre	waste water volume 3000 m ³ /d; dilution factor in receiving water 10; more realistic input concentration process water (i.e. 0,55 mg/litre) ; DT _{50,biodeg,wat/sed} is 0,71 days 25 °C (KEMI, 1995); DT _{50,biodeg,STP} is [DT _{50,biodeg,wat/sed}]/2; no hydrolysis is assumed	25
3	PEC _{surface water}	Finnish model mill 1	198	µg/litre	540 ton/d; waste water volume 800 m ³ /h (higher than normal); waste water temperature 55 °C; residence time of water 0,5 h prior to entrance STP with activated sludge; DT ₅₀ 's corrected for process temperatures	99
4	PEC _{surface water}	Finnish model mill 2	4	µg/litre	lower waste water volume than mill 1: 8740 m ³ /d (of which 60% from the short circulation of the wire part); further as mill 1; worst-case input concentration process water (i.e. 40 mg/litre) ; DT ₅₀ 's corrected for process temperatures	2,00
5	PEC _{surface water}	Finnish model mill 2	0,05	µg/litre	lower waste water volume than mill 1: 8740 m ³ /d (of which 60% from the short circulation of the wire part); further as mill 1; more realistic input concentration process water (i.e. 0,55 mg/litre) ; DT ₅₀ 's corrected for process temperatures	0,025
6	PEC _{surface water}	KEMI scenario 1	0,66	µg/litre	fine paper mill; water consumption 5000 m ³ /d; 300 m ³ white water; two dosages per day; more realistic scenario (input concentration process water 0,55 mg/litre)	0,33
7	PEC _{surface water}	KEMI scenario 2	0,088	µg/litre	newspaper mill A (2 days retention time); water consumption 25000 m ³ /d; 1000 m ³ white water; two dosages per day; more realistic scenario (input concentration process water 0,55 mg/litre)	0,04
8	PEC _{surface water}	KEMI scenario 3	0,046	µg/litre	newspaper mill B; water consumption 28000 m ³ /d; 300 m ³ white water; two dosages per day; realistic scenario (input concentration process water 0,55 mg/litre)	0,02

The abovementioned application of 5-chloro-2-methyl-4-isothiazolin-3-one is hazardous (2 of 7 refined scenarios)

Slimicide: 2,2-dithio-bis-benzamide

	PEC or PNEC	source	value	dimension	comments	PEC/PNEC
	PNEC		no data	µg/litre		
1	PEC _{surface water}	model USES (Mensink, 1999)	no data	µg/litre	waste water volume 3000 m ³ /d; dilution factor in receiving water 10; worst-case input concentration process water (i.e. X mg/litre)	no data
2	PEC _{surface water}	model USES	no data	µg/litre	waste water volume 3000 m ³ /d; dilution factor in receiving water 10; more realistic input concentration process water (i.e. Y mg/litre)	no data
3	PEC _{surface water}	Finnish model mill 1	no data	µg/litre	540 ton/d; waste water volume 800 m ³ /h (higher than normal); waste water temperature 55 °C; residence time of water 0,5 h prior to entrance WWTP with activated sludge	no data
4	PEC _{surface water}	Finnish model mill 2	no data	µg/litre	lower waste water volume than mill 1: 8740 m ³ /d (of which 60% from the short circulation of the wire part); further as mill 1; worst-case input concentration process water worst-case (i.e. X mg/litre)	no data
5	PEC _{surface water}	Finnish model mill 2	no data	µg/litre	lower waste water volume than mill 1: 8740 m ³ /d (of which 60% from the short circulation of the wire part); further as mill 1; more realistic input concentration process water (i.e. Y mg/litre)	no data
6	PEC _{surface water}	KEMI scenario 1	no data	µg/litre	fine paper mill; water consumption 5000 m ³ /d; 300 m ³ white water; two dosages per day; more realistic scenario (input concentration process water Y mg/litre)	no data
7	PEC _{surface water}	KEMI scenario 2	no data	µg/litre	newspaper mill A (2 days retention time); water consumption 25000 m ³ /d; 1000 m ³ white water; two dosages per day; more realistic scenario (input concentration process water Y mg/litre)	no data
8	PEC _{surface water}	KEMI scenario 3	no data	µg/litre	newspaper mill B; water consumption 28000 m ³ /d; 300 m ³ white water; two dosages per day; realistic scenario (input concentration process water Y mg/litre)	no data

The hazards due to the abovementioned application of 2,2-dithio-bis-benzamide are unknown

Slimicide: 5-oxo-3,4-dichloro-1,2-dithiol

	PEC or PNEC	source	value	dimension	comments	PEC/PNEC
	PNEC	KEMI, 1995; Mensink, 1999	0,014	µg/litre	PNEC based on fish (LC ₅₀ /1000); calculation conform MPC-protocol (Kalf <i>et al.</i> , 1999)	
1	PEC _{surface water}	model USES (Mensink, 1999)	3940	µg/litre	waste water volume 3000 m ³ /d; dilution factor in receiving water 10; worst-case input concentration process water (i.e. 40 mg/litre) ; no hydrolysis or degradation are assumed	281429
2	PEC _{surface water}	model USES	21	µg/litre	waste water volume 3000 m ³ /d; dilution factor in receiving water 10; more realistic input concentration process water (i.e. 0,21 mg/litre) ; no hydrolysis or degradation are assumed	1500
3	PEC _{surface water}	model USES	0,99	µg/litre	waste water volume 3000 m ³ /d; dilution factor in receiving water 10; more realistic input concentration process water (i.e. 0,21 mg/litre) ; DT _{50,hydroly} is 4,3 days; DT _{50,biodeg.wat/seed} is 0,02 days	71
4	PEC _{surface water}	Finnish model mill 1	0,00075	µg/litre	540 ton/d; waste water volume 800 m ³ /h (higher than normal); waste water temperature 55 °C; residence time of water 0,5 h prior to entrance STP with activated sludge; DT _{50,hydroly,pH5,25°C} is 54 days; DT _{50,hydroly,pH7,25°C} is 4,3 days; DT _{50,biodeg.wat/seed,pH8,25°C} is 0,02 days; DT ₅₀ 's corrected for process temperatures	0,054
5	PEC _{surface water}	Finnish model mill 2	8	µg/litre	lower waste water volume than mill 1: 8740 m ³ /d (of which 60% from the short circulation of the wire part); further as mill 1; worst-case input concentration process water worst-case (i.e. 40 mg/litre) ; DT ₅₀ 's corrected for process temperatures (for DT ₅₀ 's see calc. 3)	571
6	PEC _{surface water}	Finnish model mill 2	0,042	µg/litre	lower waste water volume than mill 1: 8740 m ³ /d (of which 60% from the short circulation of the wire part); further as mill 1; more realistic input concentration process water (i.e. 0,21 mg/litre) ; DT ₅₀ 's corrected for process temperatures (for DT ₅₀ 's see calc. 3)	3
7	PEC _{surface water}	KEMI scenario 1	0,13	µg/litre	fine paper mill; water consumption 5000 m ³ /d; 300 m ³ white water; two dosages per day; more realistic scenario (input concentration process water 0,21 mg/litre)	9
8	PEC _{surface water}	KEMI scenario 2	0,0000053	µg/litre	newspaper mill A (2 days retention time); water consumption 25000 m ³ /d; 1000 m ³ white water; two dosages per day; more realistic scenario (input concentration process water 0,21 mg/litre)	0,00038
9	PEC _{surface water}	KEMI scenario 3	0,0000051	µg/litre	newspaper mill B; water consumption 28000 m ³ /d; 300 m ³ white water; two dosages per day; realistic scenario (input concentration process water 0,21 mg/litre)	0,00036

The abovementioned application of 5-oxo-3,4-dichloro-1,2-dithiol is very hazardous (3 of 8 refined scenarios)

Slimicide: disodium cyanodithioimido carbonate

PEC or PNEC	source	value	dimension	comments	PEC/PNEC	
PNEC	EPA, 1994	0,16	µg/litre	LC ₅₀ (marine crustacean)/1000; calculation conform MPC-protocol (Kalf <i>et al.</i> , 1999)		
1	PEC _{surface water}	model USES (Mensink, 1999)	not enough data	not enough data for initial risk assessment; therefore disodium cyanodithioimidocarbonate was in the UNFAMRISK group	no data	
2	PEC _{surface water}	model USES	3970	µg/litre	waste water volume 3000 m ³ /d; dilution factor in receiving water 10; worst-case input concentration process water (i.e. 40 mg/litre) ; DT _{50,hydrol,pH7,25°C} is 7 hours; biodegradation is not assumed (no data)	24813
3	PEC _{surface water}	model USES	no data	µg/litre	waste water volume 3000 m ³ /d; dilution factor in receiving water 10; more realistic input concentration not available	no data
4	PEC _{surface water}	Finnish model mill 1	199	µg/litre	540 ton/d; waste water volume 800 m ³ /h (higher than normal); waste water temperature 55 °C; residence time of water 0,5 h prior to entrance STP with activated sludge	1244
5	PEC _{surface water}	Finnish model mill 2	530	µg/litre	lower waste water volume than mill 1: 8740 m ³ /d (of which 60% from the short circulation of the wire part); further as mill 1; worst-case input concentration process water worst-case (i.e. 40 mg/litre)	3313
6	PEC _{surface water}	Finnish model mill 2	no data	µg/litre	lower waste water volume than mill 1: 8740 m ³ /d (of which 60% from the short circulation of the wire part); further as mill 1; more realistic input concentration process water (i.e. Y mg/litre) not available	no data
7	PEC _{surface water}	KEMI scenario 1	no data	µg/litre	fine paper mill; water consumption 5000 m ³ /d; 300 m ³ white water; two dosages per day; more realistic scenario (input concentration process water Y mg/litre) not available	no data
8	PEC _{surface water}	KEMI scenario 2	no data	µg/litre	newspaper mill A (2 days retention time); water consumption 25000 m ³ /d; 1000 m ³ white water; two dosages per day; more realistic scenario (input concentration process water Y mg/litre) not available	no data
9	PEC _{surface water}	KEMI scenario 3	no data	µg/litre	newspaper mill B; water consumption 28000 m ³ /d; 300 m ³ white water; two dosages per day; more realistic scenario (input concentration process water Y mg/litre) not available	no data
10	PEC _{surface water}	EPA, 1994	2,8	µg/litre	EPA estimate for a typical sugar mill site (group A) at US mean stream flow	18
11	PEC _{surface water}	EPA, 1994	18	µg/litre	EPA estimate for a typical sugar mill site (group B) at US mean stream flow	113
12	PEC _{surface water}	EPA, 1994	1300	µg/litre	EPA estimate for an atypical sugar mill site (group A): a high exposure case, that is expected to occur once per 10 years	8125
13	PEC _{surface water}	EPA, 1994	5500	µg/litre	EPA estimate for an atypical sugar mill site (group B): a high exposure case, that is expected to occur once per 10 years	34375

The abovementioned application of disodium cyanodithioimido carbonate is very hazardous (6 of 7 refined scenarios)

Slimicide: glutaric aldehyde

	PEC or PNEC	source	value	dimension	comments	PEC/PNEC
	PNEC	KEMI, 1995; IUCLID, 1995	21	µg/litre	21-d NOEC (crustaceans)/100; calculation conform MPC-protocol (Kalf <i>et al.</i> , 1999)	
1	PEC _{surface water}	model USES	4000	µg/litre	waste water volume 3000 m ³ /d; dilution factor in receiving water 10; "worst case" input concentration process water (i.e. 40 mg/litre) , based on the max. concentration of slimicides in process water reported in ECB (1996); hydrolysis or degradation is not assumed (as data were not available)	190
2	PEC _{surface water}	model USES	633	µg/litre	waste water volume 3000 m ³ /d; dilution factor in receiving water 10; realistic-case input concentration process water (i.e. 50 mg/litre) ; K _{p,seg} and K _{p,susp mat} are 6 dm ³ /kg; DT _{50,hydroj} is 102 days; DT _{50,biodeg,wat/seg} is 0,44 days; DT _{50,biodeg,STP} is 0,029 days assuming ready biodegradability (all K _p and DT ₅₀ data from KEMI, 1995); DT _{50,biodeg,STP} appears to be crucial as a higher DT ₅₀ — e.g. 0,44/2 is 0,22 days instead of 0,029 days — increases the PEC up to 2620 µg/litre	30
3	PEC _{surface water}	Finnish model mill 1	28000	µg/litre	540 ton/d; waste water volume 800 m ³ /h (higher than normal); waste water temperature 55 °C; residence time of water 0,5 h prior to entrance STP with activated sludge; DT ₅₀ 's — see calc. 2 — corrected for process temperatures; sorption data are not used for input	1333
4	PEC _{surface water}	Finnish model mill 2	711	µg/litre	lower waste water volume than mill 1: 8740 m ³ /d (of which 60% from the short circulation of the wire part); further as mill 1; realistic input concentration process water (i.e. 50 mg/litre) ; DT ₅₀ 's — see calc. 2 — corrected for process temperatures; sorption data are not used for input	34
5	PEC _{surface water}	Finnish model mill 2	60	µg/litre	fine paper mill; water consumption 5000 m ³ /d; 300 m ³ white water; two dosages per day; realistic scenario (input concentration process water 50 mg/litre)	2,9
6	PEC _{surface water}	KEMI scenario 2	2,9	µg/litre	newspaper mill A (2 days retention time); water consumption 25000 m ³ /d; 1000 m ³ white water; two dosages per day; realistic scenario (input concentration process water 50 mg/litre)	0,14
7	PEC _{surface water}	KEMI scenario 3	2,2	µg/litre	newspaper mill B; water consumption 28000 m ³ /d; 300 m ³ white water; two dosages per day; realistic scenario (input concentration process water 50 mg/litre)	0,10

The abovementioned application of glutaric aldehyde is very hazardous (1 of 6 refined scenarios)

Slimicide: potassium N-methyldithiocarbamate

PEC or PNEC	source	value	dimension	comments	PEC/PNEC	
PNEC	Mensink, 1999	0,03	µg/litre	LC _{50,min} /1000 (0,03/1000); calculation conform MPC-protocol (Kalf <i>et al.</i> , 1999)		
1	PEC _{surface water}	model USES (Mensink, 1999)	not enough data	µg/litre	not enough data for initial risk assessment; therefore potassium N-methyldithiocarbamate was in the UNFAMRISK group	no data
2	PEC _{surface water}	model USES	1540	µg/litre	waste water volume 3000 m ³ /d; dilution factor in receiving water 10; worst-case input concentration process water (i.e. 40 mg/litre) are not available	51333
3	PEC _{surface water}	model USES	no data	µg/litre	waste water volume 3000 m ³ /d; dilution factor in receiving water 10; more realistic input concentration process water (i.e. Y mg/litre)	no data
4	PEC _{surface water}	Finnish model mill 1	276000	µg/litre	540 tonnes/day; waste water volume 800 m ³ /h (higher than normal); waste water temperature 55 °C; residence time of water 0,5 h prior to entrance STP with activated sludge; DT _{50,hydrol,pH5&7,25 °C} is assumed to be 30 days (as there are no data); then DT _{50,hydrol,55°C} is 2,7 days; DT _{50,biodeg,wat/seg} is assumed to be 60 days (as there are no data); then the DT _{50,biodeg,35°C} is 27 days, and DT _{50,biodeg,STP,35°C} is assumed to be half	9200000
5	PEC _{surface water}	Finnish model mill 2	740	µg/litre	lower waste water volume than mill 1: 8740 m ³ /d (of which 60% from the short circulation of the wire part); further as mill 1; worst-case input concentration process water worst-case (i.e. 40 mg/litre); waste water temperature 55 °C; residence time of water 0,5 h prior to entrance STP with activated sludge; DT _{50,hydrol,pH5&7,25 °C} is assumed to be 30 days (as there are no data); then DT _{50,hydrol,55°C} is 2,7 days; DT _{50,biodeg,wat/seg} is assumed to be 60 days (as there are no data); then the DT _{50,biodeg,35°C} is 27 days, and DT _{50,biodeg,STP,35°C} is assumed to be half	24667
6	PEC _{surface water}	Finnish model mill 2	no data	µg/litre	lower waste water volume than mill 1: 8740 m ³ /d (of which 60% from the short circulation of the wire part); further as mill 1; more realistic input concentration process water (i.e. Y mg/litre) not available	no data
7	PEC _{surface water}	KEMI scenario 1	no data	µg/litre	fine paper mill; water consumption 5000 m ³ /d; 300 m ³ white water; two dosages per day; more realistic scenario (input concentration process water Y mg/litre) not available	no data
8	PEC _{surface water}	KEMI scenario 2	no data	µg/litre	newspaper mill A (2 days retention time); water consumption 25000 m ³ /d; 1000 m ³ white water; two dosages per day; more realistic scenario (input concentration process water Y mg/litre) not available	no data
9	PEC _{surface water}	KEMI scenario 3	no data	µg/litre	newspaper mill B; water consumption 28000 m ³ /d; 300 m ³ white water; two dosages per day; realistic scenario (input concentration process water Y mg/litre) not available	no data

The abovementioned application of potassium N-methyldithiocarbamate is very hazardous (3 of 3 refined scenarios)

Public health area: formaldehyde

PEC or PNEC	source	value	dimension	comments	PEC/PNEC	
PNEC	IUCLID (1995)	0,3	µg/litre	EC _{50,algae} /1000; calculation conform MPC-protocol (Kalf <i>et al.</i> , 1999)		
1	PEC _{surface water}	model USES (Mensink, 1999)	0,25	µg/litre	a very general calculation for disinfectants in all accommodations without further specification; PEC a.o. based on the quantity of a.i. used in the Netherlands; default fraction of 0.002 reflect the the fraction of the total waste water in the Netherlands; DT _{50,biodeg.wat/sea} is 1 day; DT _{50,biodeg.STP} is 0,029 days (readily biodegradable)	0,83
2	PEC _{surface water}	model USES (van der Poel, 1999)	0,25	µg/litre	a more specified calculation for the sanitary sector — for private use in households — within the private and public health area disinfectants; PEC a.o. based on a calculated emission rate to waste water and not on the quantity of a.i. used in the Netherlands; DT ₅₀ 's see above	0,83
3	PEC _{surface water}	model USES (van der Poel, 1999)	2,5	µg/litre	a more specified calculation for the medical sector — for medical equipment in particular — within the private and public health area disinfectants; PEC a.o. based on a calculated emission rate to waste water and not on the quantity of a.i. used in the Netherlands; DT ₅₀ 's see above	8,3
4	PEC _{surface water}	model USES (van der Poel, 1999)	0,17	µg/litre	a more specified calculation for the medical sector — for disinfecting rooms, furniture and objects in hospitals in particular — within the private and public health area disinfectants; PEC a.o. based on a calculated emission rate to waste water and not on the quantity of a.i. used in the Netherlands; DT ₅₀ 's see above	0,57
5	PEC _{surface water}	model USES (van der Poel, 1999)	0,48	µg/litre	a more specified calculation for the medical sector — for hospital laundry in washing streets in particular — within the private and public health area disinfectants; PEC a.o. based on a calculated emission rate to waste water and not on the quantity of a.i. used in the Netherlands; DT ₅₀ 's see above	1,6
6	PEC _{surface water}	model USES (van der Poel, 1999)	0,0015	µg/litre	a more specified calculation for the medical sector — for hospital laundry in tumbler washing machines in particular — within the private and public health area disinfectants; PEC a.o. based on a calculated emission rate to waste water and not on the quantity of a.i. used in the Netherlands; DT ₅₀ 's see above	0,01

The abovementioned application of formaldehyde is hazardous (2 of 5 refined scenarios)

Public health area: glutaric aldehyde

PEC or PNEC	source	value	dimension	comments	PEC/PNEC	
PNEC	KEMI, 1995; IUCLID, 1995	21	µg/litre	21-d NOEC (crustaceans)/100; calculation conform MPC-protocol (Kalf <i>et al.</i> , 1999)		
1	PEC _{surface water}	model USES (Mensink, 1999)	1,2	µg/litre	a very general calculation for disinfectants in all accommodations without further specification; PEC a.o. based on the quantity of a.i. used in the Netherlands; default fraction of 0,002 reflect the the fraction of the total waste water in the Netherlands; hydrolysis or degradation is not assumed (as data were not available)	0,06
2	PEC _{surface water}	model USES (van der Poel, 1999)	2,1	µg/litre	a more specified calculation for the sanitary sector — for private use in households — within the private and public health area disinfectants; PEC a.o. based on a calculated emission rate to waste water and not on the quantity of a.i. used in the Netherlands; K_p , _{sed} and K_p , _{susp mat} are 6 dm ³ /kg; DT _{50,hydrol} is 102 days; DT _{50,biodeg,wat/seq} is 0,44 days; DT _{50,biodeg,STP} is 0,029 days assuming ready biodegradability (all K_p and DT ₅₀ data from KEMI, 1995); DT _{50,biodeg,STP} appears to be crucial as a higher DT ₅₀ — e.g. 0,44/2 is 0,22 days instead of 0,029 days — increases the PEC up to 2620 µg/litre	0,10
3	PEC _{surface water}	model USES (van der Poel, 1999)	178	µg/litre	a more specified calculation for the medical sector — for medical equipment in particular — within the private and public health area disinfectants; PEC a.o. based on the quantity of a.i. used in the Netherlands for disinfecting medical instruments, assuming all glutaric aldehyde is used for this purpose; for K_p and DT ₅₀ values, see above	8
4	PEC _{surface water}	model USES (van der Poel, 1999)	1,5	µg/litre	a more specified calculation for the medical sector — for medical equipment in particular — within the private and public health area disinfectants; PEC a.o. based on a default scenario for the use of 750 kg, a concentration of 80 g/litre product and a working concentration of 3,2%; for K_p and DT ₅₀ values, see above	0,07
5	PEC _{surface water}	model USES (van der Poel, 1999)	2,1	µg/litre	a more specified calculation for the medical sector — for disinfecting rooms, furniture and objects in hospitals in particular — within the private and public health area disinfectants; PEC a.o. based on a calculated emission rate to waste water and not on the quantity of a.i. used in the Netherlands; for K_p and DT ₅₀ values, see above	0,1
6	PEC _{surface water}	model USES (van der Poel, 1999)	0,64	µg/litre	a more specified calculation for the medical sector — for hospital laundry in washing streets in particular — within the private and public health area disinfectants; PEC a.o. based on a calculated emission rate to waste water and not on the quantity of a.i. used in the Netherlands; for K_p and DT ₅₀ values, see above	0,03
7	PEC _{surface water}	model USES (van der Poel, 1999)	0,0019	µg/litre	a more specified calculation for the medical sector — for hospital laundry in tumbler washing machines in particular — within the private and public health area disinfectants; PEC a.o. based on a calculated emission rate to waste water and not on the quantity of a.i. used in the Netherlands; for K_p and DT ₅₀ values, see above	0,00009

The abovementioned application of glutaric aldehyde is hazardous (1 of 6 refined scenarios)

Public health area: sodium hypochlorite

PEC or PNEC	source	value	dimension	comments	PEC/PNEC	
PNEC	IUCLID (1995) [PM, check!]	0,02	µg/litre	for total chlorine (i.e. free chlorine and chloramines) $L(E)C_{50,min}/1000 = 20/1000 = 0,02$ µg/litre; calculation conform MPC-protocol (Kalf <i>et al.</i> , 1999)		
1	PEC _{surface water}	model USES (Mensink, 1997)	40	µg/litre	a very general calculation for disinfectants in all accommodations without further specification; PEC a.o. based on the quantity of a.i. used in the Netherlands (assuming all sodium hypochlorite is used for accommodations for humans, e.g. houses, schools, hospitals, offices); default fraction of 0.002 reflect the fraction of the total waste water in the Netherlands; no hydrolysis and biodegradation are assumed (as no data were available; unrealistic worst case)	2000
2	PEC _{surface water}	model USES (van der Poel, 1999)	12	µg/litre	a more specified calculation for the sanitary sector — for private use in households — within the private and public health area disinfectants; PEC a.o. based on a calculated emission rate to waste water and not on the quantity of a.i. used in the Netherlands; $DT_{50,hydra1}$ is arbitrarily 0,01 days; $DT_{50,biodeg,wat/seed}$ is arbitrarily 0,01 days; $DT_{50,biodeg,STP}$ is 0,029 days assuming ready biodegradability	600
3	PEC _{surface water}	model USES (van der Poel, 1999)	0,59	µg/litre	a more specified calculation for the medical sector — for disinfecting rooms, furniture and objects in hospitals in particular — within the private and public health area disinfectants; PEC a.o. based on a calculated emission rate to waste water and not on the quantity of a.i. used in the Netherlands; partitioning based on a "log Kow" of -1; the substance is readily biodegradable in an STP; $DT_{50,hydra1}$ and $DT_{50,biodeg,wat/seed}$ are 1 day	30

The abovementioned application of sodium hypochlorite is very hazardous (1 of 2 refined scenarios)

Public health area: potassium hydroxide

PEC or PNEC	source	value	dimension	comments	PEC/PNEC	
PNEC	IUCLID (1995)	80	µg/litre	LC _{50,min,fish} /1000; calculation conform MPC-protocol (Kalf <i>et al.</i> , 1999)		
1	PEC _{surface water}	model USES (Mensink, 1999)	not enough data	not enough data for initial risk assessment; therefore potassium hydroxide was in the UNFAMRISK group	no data	
2	PEC _{surface water}	model USES (Linders & Jager, 1997)	82	µg/litre	a very general calculation for disinfectants in all accommodations without further specification; PEC a.o. based on the quantity of a.i. used in the Netherlands (335,000 kg/year); default fraction of 0,002 reflect the the fraction of the total waste water in the Netherlands	1,0
3	PEC _{surface water}	model USES (Linders & Jager, 1997)	0,061	µg/litre	a very general calculation for disinfectants in all accommodations without further specification; PEC a.o. based on the default quantity of a.i. used in the Netherlands (250 kg/year); default fraction of 0,002 reflect the the fraction of the total waste water in the Netherlands	0,0008
4	PEC _{surface water}	model USES (van der Poel, 1999)	167000	µg/litre	a more specified calculation for the medical sector — for medical equipment in particular — within the private and public health area disinfectants; PEC a.o. based on a calculated emission rate to waste water and on the quantity of a.i. used in the Netherlands	2088

The abovementioned application of potassium hydroxide is non-hazardous (1 of 2 refined scenarios; scenario 4 is considered unrealistic)

Public health area: sodium dichloroisocyanurate

PEC or PNEC	source	value	dimension	comments	PEC/PNEC	
PNEC	IUCLID (1995)	0,13	µg/litre	LC _{50,fish} /1000; calculation conform MPC-protocol (Kalf <i>et al.</i> , 1999)		
1	PEC _{surface water}	model USES (Mensink, 1999)	9,2	µg/litre	a very general calculation for disinfectants in all accommodations without further specification; PEC a.o. based on the quantity of a.i. used in the Netherlands (assuming all sodium dichloroisocyanurate is used for accommodations for humans e.g. houses, schools, hospitals, offices). default fraction of 0.002 reflect the the fraction of the total waste water in the Netherlands; no hydrolysis or degradation is assumed	71
2	PEC _{surface water}	model USES (Linders & Jager, 1997)	2640	µg/litre	a general calculation for use in a swimming pool that discharges two times per year; DT _{50,hydrolysis} is assumed to be 1 d (forming hypochlorous acid and cyanuric acid); the swimming pool contains 100 mg cyanuric acid/litre — the maximum amount in accordance with user's instructions — which is equivalent to 171 mg sodium dichloroisocyanurate; emission rate to STP is 135 kg/day	20308
3	PEC _{surface water}	model USES (van der Poel, 1999)	70	µg/litre	a more specified calculation for the medical sector — for disinfecting rooms, furniture and objects in hospitals in particular — within the private and public health area disinfectants; PEC a.o. based on a calculated emission rate to waste water and not on the quantity of a.i. used in the Netherlands	538
4	PEC _{surface water}	model USES (van der Poel, 1999)	400	µg/litre	a more specified calculation for the medical sector — for hospital laundry in washing streets in particular — within the private and public health area disinfectants; PEC a.o. based on a calculated emission rate to waste water and not on the quantity of a.i. used in the Netherlands	3077
5	PEC _{surface water}	model USES (van der Poel, 1999)	1,3	µg/litre	a more specified calculation for the medical sector — for hospital laundry in tumbler washing machines in particular — within the private and public health area disinfectants; PEC a.o. based on a calculated emission rate to waste water and not on the quantity of a.i. used in the Netherlands	10

The abovementioned application of sodium dichloroisocyanurate is very hazardous (3 of 4 refined scenarios)

Public health area:

sodium p-toluenesulfonchloramide

PEC or PNEC	source	value	dimension	comments	PEC/PNEC	
PNEC	IUCLID (1995)	22	µg/litre	NOEC _{min} /50 = 1100/50 = 22 µg/litre; calculation conform MPC-protocol (Kalf <i>et al.</i> , 1999)		
1	PEC _{surface water}	model USES (Mensink, 1999)	17	µg/litre	a very general calculation for disinfectants in all accommodations without further specification; PEC a.o. based on the quantity of a.i. used in the Netherlands (assuming all sodium p-toluenesulfonchloramide is used for accommodations for humans, e.g. houses, schools, hospitals, offices); default fraction of 0,002 reflect the the fraction of the total waste water in the Netherlands; no hydrolysis or degradation is assumed	0,77
2	PEC _{surface water}	model USES (Linders & Jager, 1997)	1	µg/litre	a very general calculation for disinfectants in all accommodations without further specification; PEC a.o. based on the quantity of a.i. used in the Netherlands; default fraction of 0,002 reflect the the fraction of the total waste water in the Netherlands; assuming ready hydrolysis (DT _{50,hydrolyt} 2 days) and inherent biodegradability, fulfilling specific criteria	0,05
3	PEC _{surface water}	model USES (van der Poel, 1999)	118	µg/litre	a more specified calculation for the sanitary sector — for private use in households — within the private and public health area disinfectants; PEC a.o. based on a calculated emission rate to waste water and not on the quantity of a.i. used in the Netherlands; assuming inherent biodegradability, fulfilling specific criteria	5
4	PEC _{surface water}	model USES (van der Poel, 1999)	12	µg/litre	a more specified calculation for the medical sector — for disinfecting rooms, furniture and objects in hospitals in particular — within the private and public health area disinfectants; PEC a.o. based on a calculated emission rate to waste water and not on the quantity of a.i. used in the Netherlands; assuming inherent biodegradability, fulfilling specific criteria	0,55
5	PEC _{surface water}	model USES (van der Poel, 1999)	35	µg/litre	a more specified calculation for the medical sector — for hospital laundry in washing streets in particular — within the private and public health area disinfectants; PEC a.o. based on a calculated emission rate to waste water and not on the quantity of a.i. used in the Netherlands; assuming inherent biodegradability, fulfilling specific criteria	1,6
6	PEC _{surface water}	model USES (van der Poel, 1999)	0,11	µg/litre	a more specified calculation for the medical sector — for hospital laundry in tumbler washing machines in particular — within the private and public health area disinfectants; PEC a.o. based on a calculated emission rate to waste water and not on the quantity of a.i. used in the Netherlands; assuming inherent biodegradability, fulfilling specific criteria	0,005

The abovementioned application of sodium p-toluenesulfonchloramide is "disputably" hazardous (2 of 5 refined scenarios)

Wood preservatives: arsenic pentoxide

PEC or PNEC	source	value	dimension	comments	PEC/PNEC	
PNEC	Crommentuijn <i>et al.</i> , 1997	24	µg/litre	This PNEC is the Maximum Permissible Addition (MPA). Adding this MPA to the natural background levels gives the Maximum Permissible Concentration.		
1	PEC _{surface water}	model USES (Mensink, 1999)	0,33	µg/litre	This PEC is calculated for a standard impregnation facility discharging its waste water on an STP. The concentration in the wood is 6,5 kg.m ³ — see the product profile of KEMWOOD CCA-C in Mensink (1999). The K _d of the sludge in the STP is assumed to be 6607 dm ³ /kg (conform Crommentuijn <i>et al.</i> , 1997)	0,01
2	PEC _{surface water}	model USES	24	µg/litre	Exposure from sheet piles in a model ditch. The mean flux of As is arbitrarily assumed to be 0,48% over a period of 1 year: then, a concentration in the wood of 6,5 kg/m ³ wood — see the product profile in Mensink (1999) — gives a mean flux of 2,2 mg.m ⁻² .day ⁻¹ . This flux — from 4,7 m ² sheet pile per meter model waterway equalling 0,12 m ³ wood — gives an initial PEC of 24 µg/litre, assuming momentaneous partitioning to suspended matter (0,015 kg/litre) with a K _d of 10000 dm ³ /litre (conform Crommentuijn <i>et al.</i> , 1997). This calculation shows that a flux of 0,48% is a cutoff value whether the PEC/PNEC of 1 will be exceeded or not. However, there is no clarity yet, whether the actual flux will exceed this cutoff flux or not (person. communic. CTB to RIVM), pending the discussion in the first quarter of 2000 on banning CCA salts or not. There are no reliable monitoring data to verify these model calculations (Smit & Montforts, 1998).	1

The abovementioned application of arsenic pentoxide is non-hazardous (1 of 2 scenarios) or the hazard is unknown (1 of 2 scenarios)

Wood preservatives: 2-methyl-4-isothiazolin-3-one

PEC or PNEC	source	value	dimension	comments	PEC/PNEC	
PNEC	KEMI, 1995; EPA, 1998; Mensink, 1999	0,7	µg/litre	PNEC based on the lowest of two chronic MATCs (crustaceans & fish) (MATC/50); calculation conform MPC-protocol (Kalf <i>et al.</i> , 1999)		
1	PEC _{surface water}	model USES (Mensink, 1999)	3	µg/litre	This PEC is calculated for a standard impregnation facility discharging its waste water on an STP. Hydrolysis or degradation is not assumed (as no data were available); sorption data were also not available	4,3
2	PEC _{surface water}	model USES	0,00008	µg/litre	This PEC is calculated for a standard impregnation facility discharging its waste water on an STP. The minimum concentration in the wood is 1,1 g.m³ —see the product profile of TANAMIX 3743 in Mensink (1999). 2-methyl-4-isothiazolin-3-one has a DT _{50,biodeg,wat/seq} of 0,38 days (KEMI, 1995); DT _{50,biodeg,STP} is arbitrarily assumed to be [DT _{50,biodeg,wat/seq}]/2; K _{om,sus mat} is 309 dm ³ /kg (derived from a K _{oc,seq} of 310 dm ³ /kg for 5-chloro-2-methyl-4-isothiazolin-3-one in EPA, 1998)	0,0001
3	PEC _{surface water}	model USES	0,00014	µg/litre	This PEC is calculated for a standard impregnation facility discharging its waste water on an STP. The maximum concentration in the wood is 1,9 g.m³ —see the product profile of TANAMIX 3743 in Mensink (1999). 2-methyl-4-isothiazolin-3-one has a DT _{50,biodeg,wat/seq} of 0,38 days (KEMI, 1995); DT _{50,biodeg,STP} is arbitrarily assumed to be [DT _{50,biodeg,wat/seq}]/2; K _{om} see above	0,0002
4	PEC _{surface water}	model USES	0,16	µg/litre	Exposure from sheet piles in a model ditch; this ditch contains 15 mg suspended matter per litre; K _{om,susp matter} is 309 dm ³ /kg (derived from a K _{oc,sediment} of 310 dm ³ /kg for 5-chloro-2-methyl-4-isothiazolin-3-one in EPA, 1998); it is arbitrarily assumed that 10% of the impregnated amount leaches within one year of other wood preservatives used for sheet piling). 2-methyl-4-isothiazolin-3-one has a DT _{50,biodeg,wat/seq} of 0,38 days (KEMI, 1995); K _{om} see above	0,23
5	PEC _{surface water}	model USES	18	µg/litre	Exposure from sheet piles in a model ditch; this ditch contains 15 mg suspended matter per litre; K _{om,sus mat} see above; it is assumed that 84% of the impregnated amount leaches within 28 days (as reported for pine wood blocks in seawater by EPA, 1998). 2-methyl-4-isothiazolin-3-one has a DT _{50,biodeg,wat/seq} of 0,38 days (KEMI, 1995)	26

The abovementioned application of 2-methyl-4-isothiazolin-3-one is hazardous (1 of 4 refined scenarios)

Wood preservatives: dichlofluanide

PEC or PNEC	source	value	dimension	comments	PEC/PNEC	
PNEC	see comments	30	µg/litre	PNEC is the Maximum Permissible Concentration (CIW/CUWVO, 1999). However, this MPC is not reported in the final decision document of the Dutch government (V&W, 1998). Therefore, its current legislative status is not clear. Probably, it should be seen as an <i>ad hoc</i> MPC. Based on the data in Mensink (1999), the PNEC should be $LC_{50, fish, min} / 1000$ which is 0,05 µg/litre. It is difficult to compare this PNEC with the <i>ad hoc</i> MPC. Until further notice the <i>ad hoc</i> MPC will be preferred.		
1	PEC _{surface water}	model USES (Mensink, 1999)	0,32	µg/litre	Exposure during wood processing in a standard impregnating plant after treatment in a municipal sewage treatment plant. The impregnated amount is assumed to be 2 kg.m ⁻³ (default), dichlofluanide is not assumed to be hydrolysable or biodegradable (as data were not available)	0,011
2	PEC _{surface water}	model USES	0,62	µg/litre	Exposure during wood processing in a standard impregnating plant after treatment in a municipal sewage treatment plant. The impregnated amount is assumed to be 30 kg.m ⁻³ (max. amount for EMBASOL DT). Dichlofluanide is assumed to be readily biodegradable (in view of the EPIWIN estimate). However, even in the case of assuming no biodegradability — giving a PEC _{surface water} of 4,8 µg/litre — the PNEC would not be exceeded (with an RCR of 0,16)	0,021

The abovementioned application of dichlofluanide is non-hazardous (1 of 1 refined scenario)

Wood preservatives: 5-chloro-2-methyl-4-isothiazolin-3-one

PEC or PNEC	source	value	dimension	comments	PEC/PNEC	
PNEC	KEMI, 1995; EPA, 1998; Mensink, 1999	2	µg/litre	PNEC based on 2 additional NOECs for different taxonomic groups: 0,10/50; calculation conform MPC-protocol (Kalf <i>et al.</i> , 1999)		
1	PEC _{surface water}	model USES (Mensink, 1999)	0,33	µg/litre	This PEC is calculated for a standard impregnation facility discharging its waste water on an STP. Hydrolysis or degradation is not assumed (as no data were available), sorption data were also not available	0,17
2	PEC _{surface water}	model USES	0,00025	µg/litre	This PEC is calculated for a standard impregnation facility discharging its waste water on an MSTP. The minimum concentration in the wood is 3,4 g.m³ —see the product profile of TANAMIX 3743 in Mensink (1999); DT _{50,biodeg,wat/sed} is 0,72 days (KEMI, 1995); DT _{50,biodeg,STP} is arbitrarily assumed to be [DT _{50,biodeg,wat/sed}]/2; K _{p,sus mat} and K _{p,sed} are 26 and 16 dm ³ /kg, respectively	0,0001
3	PEC _{surface water}	model USES	0,00044	µg/litre	This PEC is calculated for a standard impregnation facility discharging its waste water on an MSTP. The maximum concentration in the wood is 5,9 g.m³ —see the product profile of TANAMIX 3743 in Mensink (1999); for K _p and DT ₅₀ 's see above	0,0002
4	PEC _{surface water}	model USES	0,42	µg/litre	Exposure from sheet piles in a model ditch; this ditch contains 15 mg suspended matter per litre; K _{om,susp matter} is 309 dm ³ /kg (derived from a K _{oc,sediment} of 310 dm ³ /kg in EPA, 1998); it is arbitrarily assumed that 10% of the impregnated amount leaches within one year <i>cf</i> other wood preservatives used for sheet piling); for K _p and DT ₅₀ 's see above	0,21
5	PEC _{surface water}	model USES	47	µg/litre	Exposure from sheet piles in a model ditch; this ditch contains 15 mg suspended matter per litre; K _{om,susp matter} is 309 dm ³ /kg (derived from a K _{oc,sediment} of 310 dm ³ /kg in EPA, 1998); it is assumed that 84% of the impregnated amount leaches within 28 days (as reported for pine wood blocks in seawater by EPA, 1998); for K _p and DT ₅₀ 's see above	24

The abovementioned application of 5-chloro-2-methyl-4-isothiazolin-3-one is hazardous (1 of 4 refined scenarios)

Wood preservatives: potassium bifluoride

	PEC or PNEC	source	value	dimension	comments	PEC/PNEC
	PNEC		no data	µg/litre		no data
1	PEC _{surface water}	model USES (Mensink, 1999)	no data	µg/litre	not enough data for initial risk assessment, therefore potassium bifluoride was in the UNFAMRISK group	no data
2	PEC _{surface water}		0	µg/litre	Exposure during wood processing in a standard impregnating plant after treatment in a municipal sewage treatment plant	0
3	PEC _{surface water}		not relevant	µg/litre	Exposure from sheet piles in a model ditch	not relevant

The registration of IMPROSOL — a biocide to preserve front carpentry by dipping the wood in a special installation — has not been continued since 01-03-2000 as the appropriate company has not asked for reregistration. The other product with F₂HK — WOODPIL, a plug that is made by compressing dry powders of ammonium bifluoride and potassium bifluoride — has the same expiration date. However, the appropriate company has asked the National Board for the Authorisation of Pesticides for reregistration (person. communic. of WOODCAP BV to RIVM). As the making of plugs is a dry process, no emissions to the environment are expected. The Board has asked the appropriate company to provide data on the leaching behaviour of ammonium and potassium bifluoride from front carpentry during a period of 100 days as a requirement for reregistration. It should be noted that the biocidal action is probably by HF released by F₂HK under relatively moist conditions that otherwise would promote wood decay, and as both HF and F₂HK are reactive compounds, emissions to the environment does not seem likely.

The abovementioned application of potassium bifluoride is non-hazardous (1 of 1 scenario)

Wood preservatives: cupric carbonate hydroxide

PEC or PNEC	source	value	dimension	comments	PEC/PNEC	
PNEC	Crommentuijn <i>et al.</i> , 1997	1,1	µg/litre	This PNEC is the Maximum Applicable Addition (MAA). Adding this MAA to the natural background levels gives the Maximum Applicable Concentration.		
1	PEC _{surface water}	model USES (Mensink, 1999)	0,33	µg/litre	This PEC is calculated for a standard impregnation facility discharging its waste water on an STP. Concentration in the wood is 2 kg/m ³ (default). Hydrolysis or degradation is not assumed (as no data were available); sorption data were also not available	0,30
2	PEC _{surface water}	model USES	0,16	µg/litre	This PEC is calculated for a standard impregnation facility discharging its waste water on an STP. The concentration in the wood is 8 kg/m ³ — see the product profile of TANALIT E in Mensink (1999). The K _p of the sludge in the MSTP is assumed to be the K _{p, sed} from Crommentuijn <i>et al.</i> , 1997 (33884 dm ³ /kg)	0,15
3	PEC _{surface water}	model USES	1,1	µg/litre	Exposure from sheet piles in a model ditch. The mean flux of Cu is arbitrarily assumed to be 10% over a period of 1 year: then, a concentration in the wood of 8 kg/m ³ wood — see the product profile of TANALIT E in Mensink (1999) — gives a mean flux of 56 mg.m ⁻² .day ⁻¹ . This flux — from 4,7 m ² sheet pile per meter waterway equalling 0,12 m ³ wood — gives an initial PEC of 402 µg/litre, assuming momentaneous partitioning to suspended matter (0,015 kg/litre) with a K _{p, sus mat} of 50119 dm ³ /litre (conform Crommentuijn <i>et al.</i> , 1997). An additional calculation shows that a flux of 0,027% is a cutoff value whether the PEC/PNEC of 1 will be exceeded or not. It was, however, beyond the scope of this project, to verify this flux percentage	1

The abovementioned application of cupric carbonate hydroxide is non-hazardous (1 of 2 refined scenarios) or the hazard is unknown (1 of 2 refined scenario's)

Liquid cooling system preservative: 2,2-dibromo-3-nitrilopropionamide

PEC or PNEC	source	value	dimension	comments	PEC/PNEC	
PNEC	KEMI, 1995; Mensink, 1999	0,3	µg/litre	PNEC based on algae (EC ₅₀ /1000); calculation conform MPC-protocol (Kalf <i>et al.</i> , 1999)		
1	PEC _{surface water}	model USES	120	µg/litre	PEC is based on 0,5 mg a.l./litre cooling water (default); DT _{50,hydrol} is 1,5 day (as other data were not available); no other routes of dissipation; no sorption data	400
2	PEC _{surface water}	model USES	8700	µg/litre	PEC is the concentration in the blow-down of an open circulating cooling system; the concentration in the process water is 26 mg/litre (see the product file of BACTERICIDE 440 in Mensink, 1999); the substance is readily hydrolysing with a DT _{50,hydrol} of 2,6 days at pH 5; the substance is readily biodegradable; no STP; K _{p,sus.mat} is 4,6 dm ³ /kg (based on K _{oc,soil} of 32 dm ³ /kg)	29000
3	PEC _{surface water}	model USES	4677	µg/litre	PEC is the concentration in the blow-down of an open circulating cooling system; the concentration in the process water is 14 mg/litre (see the product file of BIOBROM C-103-L in Mensink, 1999); the substance is readily hydrolysing with a DT _{50,hydrolysis} of 2,6 days at pH 5; the substance is readily biodegradable; no STP	15590
4	PEC _{surface water}	model USES	836	µg/litre	PEC is the concentration in the blow-down of an open circulating cooling system; the concentration in the process water is 2,5 mg/litre (see the product file of AQUACID DSB in Mensink, 1999); the substance is readily hydrolysing with a DT _{50,hydrolysis} of 2,6 days at pH 5; the substance is readily biodegradable; no STP	2787

2,2-dibromo-3-nitrilopropionamide was determined in acidified samples — to prevent hydrolysis — from the sluice in the tank under the cooling tower of a Dutch energy plant (Baltus *et al.*, 1999). These samples showed that the concentration of the parent compound and its probable hydrolysis product were max. 12 and 18 mg/litre, respectively (analysis 2 days after sampling). These concentrations exceed the PNEC up to 40000 times. However, the blow-down was sampled prior to a biological treatment before discharging on the surface water. Therefore these figures are difficult to compare with the calculations above. However, in all cases, PECs, whether calculated or measured, appear to exceed the PNECs substantially.

The abovementioned application of 2,2-dibromo-3-nitrilopropionamide is very hazardous (3 of 3 refined scenarios)

Liquid cooling system preservative: 2-methyl-4-isothiazolin-3-one

PEC or PNEC	source	value	dimension	comments	PEC/PNEC	
PNEC	KEMI, 1995; EPA, 1998; Mensink, 1999	0,7	µg/litre	PNEC based on the lowest of two chronic MATCs (crustaceans & fish) (MATC/50); calculation conform MPC-protocol (Kalf <i>et al.</i> , 1999)		
1	PEC _{surface water}	model USES (Mensink, 1999)	170	µg/litre	PEC is based on 0,5 mg a.l./litre cooling water (default); no hydrolysis or degradation was assumed (as data were not available); no sorption data	243
2	PEC _{surface water}	model USES	189	µg/litre	PEC is the concentration in the blow-down of an open circulating cooling system; the concentration in the proces water is 0,57 mg/litre (see the product file of PIROR P-1045 in Mensink, 1999); no hydrolysis; DT _{50,biodeg,wat/sed} is 0,38 days; K _{om,sus mat} is 309 dm ³ /kg (derived from a K _{oc, sed} of 310 dm ³ /kg for 5-chloro-2-methyl-4-isothiazolin-3-one in EPA, 1998); no STP	270
3	PEC _{surface water}	model USES	1525	µg/litre	PEC is the concentration in the blow-down of an open circulating cooling system; the concentration in the proces water is 4,6 mg/litre (see the product file of ACTICIDE 14 in Mensink, 1999); no hydrolysis; DT _{50,biodeg,wat/sed} is 0,38 days; for K _{om} see above; no STP	2179

The abovementioned application of 2-methyl-4-isothiazolin-3-one is very hazardous (2 of 2 refined scenarios)

Liquid cooling system preservative: 5-chloro-2-methyl-4-isothiazolin-3-one

PEC or PNEC	source	value	dimension	comments	PEC/PNEC	
PNEC	KEMI, 1995; EPA, 1998; Mensink, 1999	2	µg/litre	PNEC based on 2 additional NOECs for different taxonomic groups: 0,10/50; calculation conform MPC-protocol (Kalf <i>et al.</i> , 1999)		
1	PEC _{surface water}	model USES (Mensink, 1999)	170	µg/litre	PEC is based on 0,5 mg a.l./litre cooling water (default); no hydrolysis or degradation was assumed (as data were not available); no sorption data	85
2	PEC _{surface water}	model USES	530	µg/litre	PEC is the concentration in the blow-down of an open circulating cooling system; the concentration in the proces water is 1,6 mg/litre (see the product file of PIROR P-1045 in Mensink, 1999); no hydrolysis; DT _{50,biodeg,water} is 0,72 days (KEMI, 1995); K _{p,sus mat} and K _{p,sed} are 26 and 16 dm ³ /kg, respectively; no STP	265
3	PEC _{surface water}	model USES	3942	µg/litre	PEC is the concentration in the blow-down of an open circulating cooling system; the concentration in the proces water is 11,9 mg/litre (see the product file of ACTICIDE 14 in Mensink, 1999); no hydrolysis; for K _p and DT ₅₀ 's see above; no STP	1971

The abovementioned application of 5-chloro-2-methyl-4-isothiazolin-3-one is very hazardous (2 of 2 refined scenarios)

Liquid cooling system preservative: glutaric aldehyde

PEC or PNEC	source	value	dimension	comments	PEC/PNEC	
PNEC	KEMI, 1995; IUCLID, 1995	21	µg/litre	21-d NOEC (crustaceans)/100; calculation conform MPC-protocol (Kalf <i>et al.</i> , 1999)		
1	PEC _{surface water}	model USES	167	µg/litre	PEC is the concentration in the blow-down of an open circulating cooling system; the concentration in the proces water is 0.5 mg/litre (default); hydrolysis or degradation is not assumed (as data were not available).	8
2	PEC _{surface water}	model USES	34000	µg/litre	PEC is the concentration in the blow-down of an open circulating cooling system; the concentration in the proces water is 102 mg/litre (see the product files of AQUICAR (R) and AQUICAR 550 in Mensink, 1999); DT _{50,biodeg,wat/sed} is 0,44 days; K _{p,sed} and K _{p,susp.mat} are 6 dm ³ /kg; DT _{50,hydrol} is 102 days; no STP	1619

The abovementioned application of glutaric aldehyde is very hazardous (1 of 1 refined scenario)

Liquid cooling system preservative: sodium hypochlorite

PEC or PNEC	source	value	dimension	comments	PEC/PNEC	
PNEC	IUCLID (1995)	0,02	µg/litre	for total chlorine (<i>i.e.</i> free chlorine and chloramines) L(E)C _{50,min} /1000 = 20/1000 = 0,02 µg/litre; calculation conform MPC-protocol (Kalf <i>et al.</i> , 1999)		
1	PEC _{surface water}	model USES (Mensink, 1999)	170	µg/litre	PEC is based on 0.5 mg a.i./litre cooling water (default); log K _{ow} assumed to be -1 (this is a pseudo K _{ow} , as USES is actually not appropriate for inorganic substances; however, no proper sorption data are available, otherwise these could have been the substitutes of those calculated on the basis of log K _{ow} with a QSAR; no hydrolysis or degradation was assumed (as data were not available)	8500
2	PEC _{surface water}	model USES	6670	µg/litre	PEC calculated for a continuous flow system with SPECTRUS OX 1272; log K _{ow} assumed to be -1; concentration in process water is assumed to be 20 mg a.i./litre; DT _{50,biodeg,water/sed} and DT _{50,hydroly} are arbitrarily assumed to be 0.01 day; direct discharge on surface water	333500

The abovementioned application of sodium hypochlorite is very hazardous (1 of 1 refined scenario)

Appendix 4 Mailing list

- 1 Directoraat-Generaal Milieubeheer, Directeur Bodem, Water en Landelijk gebied, drs. J.A. Suurland
- 2 Directoraat-Generaal Milieubeheer, Directeur Stoffen, Veiligheid en Straling, dr. C.M. Plug
- 3 plv. Directeur-Generaal Milieubeheer, dr. ir. B.C.J. Zoeteman
- 4 Directoraat-Generaal Milieubeheer, Directie Bodem, Water en Landelijk gebied, drs. H. Merkus
- 5 Directoraat-Generaal Milieubeheer, Directie Bodem, Water en Landelijk gebied, mw. dr. J.W. Tas
- 6 prof. dr. J.S.M. Boleij, CTB
- 7 mw. drs. B. de Heer, Inter Provinciaal Overleg
- 8 mw. drs. ing. C.A.M. Baltus, RIZA
- 9 dr. R.H. Jellema, CBS, postbus 4000, 2270 JM Voorburg
- 10 drs. H.A.W. Kleinjans, Ameco
- 11 dhr. J. Bouwma, VNCI
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- 18 Clustercoördinator Milieukwaliteit, ir. R. van den Berg
- 19 Hoofd Centrum voor Stoffen en Risicobeoordeling, dr. W.H. Könemann
- 20 Hoofd Laboratorium voor Water- en Drinkwateronderzoek, dr. A.H.M. Bresser
- 21 prof. dr. C.J. van Leeuwen, CSR
- 22 ir. P.T.J. van der Zandt, CSR
- 23 mw. ir. M. Hof, CSR
- 24 ir. J.B.H.J. Linders, CSR
- 25 drs. R. Luttik, CSR
- 26 drs. M.H.M.M. Montforts, CSR
- 27 ing. P. van der Poel, CSR
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