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Assessment of the consequences of a possible ban on phosphates in household detergents

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Content

Introduction

Based on the Detergent Directive Article 16 the EU Commission may release a proposal on limitation on usage of phosphates in household detergents. A similar proposal is part of the HELCOM Baltic Sea Action Plan.

So far, the Danish opinion has been that the regulation should take place at a national level. The reason given by the Danish Environmental Agency is that discharge of phosphates in Denmark is efficiently limited by the wastewater treatment and information on the environmental impact of the alternative substances is missing.

This project focuses on the consequences of a possible ban of phosphate in laundry detergents but includes also consequences of a possible ban of phosphate in automatic dishwashing products. The project identifies substances for substitution of phosphate in laundry and automatic dishwashing detergents and includes an ecotoxicological risk assessment of selected substitutes. The consequences on the wastewater treatment from the substitution of phosphate and the increased use of the alternative substances are evaluated.

The project was preformed by DHI. The project group consisted of Torben Madsen, Kim Gustavson, Tina Slothuus, Anne Rathmann Pedersen, Ulf Nielsen and Kenneth Frants Janning.

Sammenfatning og konklusioner

Et forslag til begrænsninger i brugen af fosfat i vaskemidler kan blive fremsat af EU Kommissionen eller blive fremsat som del af HELCOM Østersøaktionsplanen. Formålet med dette projekt er at foretage en miljøeffektvurdering af potentielle erstatningsstoffer til fosfat i vaskemidler og vurdere konsekvenserne af erstatning af fosfat og øget brug af erstatningsstofferne på processerne i renseanlæg.

Projektet identificerer erstatningsstoffer for fosfat i tekstilvaskemidler og i maskinopvaskemidler. De vigtigste erstatningsstoffer for fosfat i vaskemidler er zeoliter, polykarboxylater, citrater og fosfonater. Nye alternativer som IminoDiSuccinate (IDS), Methyl Glycin Diacetic Acid (MGDA) og GLutamic acid Diacetic Acid (GLDA) er også introduceret i buildersystemer i dag men i et mindre omfang. De vigtigste alternativer til fosfat i maskinopvaskemidler er citrater, silikater og karbonater.

Miljøvurderingen af effekter på det akvatiske miljø blev udført som en trinvis proces. Effektvurderingen omfatter ikke effekter i det terrestriske miljø. Først blev der foretaget en indledende screening til identifikation af stoffer med det højeste miljøfarlighedspotentiale. Screeningen var baseret på typiske koncentrationer af fosfaterstatningsstofferne i tekstilvaskemidler og maskinopvaskemidler. Parametre fra Detergent Ingredients Database list (DID list) fra de europæiske og nordiske miljømærkeordninger blev anvendt til at beregne et risikoindeks, der udtrykker stoffets miljøfarlighedspotentiale. For stofferne med den højeste potentielle miljøfarlighed blev Predicted Environmental Concentrations, PEC bestemt ved hjælp af to forskellige metoder: EUSES og ECO Lab modellering. Økotoksikologiske data blev fundet i tilgængelige databaser og Predicted No-Effect Concentrations ($PNEC_{aquatic}$) blev udledt i henhold til principperne i EU's Technical Guidance Document for risikovurdering (TGD). Som resultat af miljørisikovurderingen blev risikokvotienten, RQ (PEC/PNEC) bestemt for kronisk såvel som akut eksponering.

Screeningen identificerer natriumsilikat og zeolit som erstatningsstoffer for fosfat i tekstilvaskemidler med den højeste potentielle miljøfarlighed. For maskinopvaskemidlerne er natriumsilikat fosfatalternativet med den højeste potentielle miljøfarlighed baseret på resultatet i screeningen.

En miljøvurdering for det akvatiske miljø blev udført for natriumsilikat, zeolit, fosfonater og IDS (Iminodisuccinat) med fokus på deres brug som fosfatalternativer i tekstilvaskemidler. RQ, som blev beregnet for kronisk og akut eksponering, blev alle beregnet til at være under 1 indikerende, at brugen af fosfaterstatningsstofferne i tekstilvaskemidler ikke forventes at udgøre en risiko i det akvatiske miljø.

Konsekvensen for renseanlæggenes funktion og effektivitet som følge af en reduceret fosforbelastning og stigende tilløbsbelastning af erstatningsstoffer for fosfor blev evalueret.

Beregningen af fosforbelastningen til danske rensningsanlæg er bestemt ved at udregne husholdningsforbruget af vaskemidler i Danmark. Sammenlignet med Miljøstyrelsens nøgletal for brug af sæbestoffer i husholdningen fås et væsentligt større vaskemiddelforbrug (51,751 tons vaskemiddel/år) mod MST, 2001 (28,700 tons/år). Sammenlignes med Danmarks Statistik ligger begge estimater dog væsentligt lavere, idet Danmarks Statistik har opgjort et forbrug på 78,364 tons vaskemidler/år, hvorfor det må konkluderes, at der er meget stor usikkerhed på bestemmelserne af det reelle vaskemiddelforbrug i Danmark.

Ved introduktion af et forbud mod brugen af fosfatholdige tekstil- og maskinopvaskemidler i private husholdninger vil niveauet for tilledning af fosfor til kommunale renseanlæg falde betydeligt. I dag indeholder 60-70% af tekstilvaskemidler og 100% af maskinopvaskemidler stadig fosfater[1]. Såfremt det antages, at der i danske husholdninger forbruges 51,751 tons vaskemiddel/år, estimeres det, at reduktionen i fosforbelastningen til renseanlæggene kunne blive op til 46% - en reduktion, der svarer til 2.450 tons fosfor per år. Fosfor indløbskoncentrationsniveauet til renseanlæg ville dermed i gennemsnit blive reduceret fra 8,9 mg P/l til 4,8 mg P/l som følge af en fuld fosfor substitution i husholdningsvaskemidlerne.

Effekten af dette vil være omfattende for renseanlæggenes drift, idet det sandsynligvis vil resultere i en næsten fuldstændig reduktion i behovet for kemisk fældning, som i dag fjerner 30-40% af fosforen i renseanlæggene, og som er ansvarlig for en stor del af slamproduktionen på danske renseanlæg. Dette vil i praksis også resultere i betydelige driftsbesparelser i forhold til brugen af fældningskemikalier i en størrelsesorden der mindst andrager 50 mio. DKK. Der kan dog blive behov for procesomlægninger samt ombygning af renseanlæggene. Det lavere indhold af fosfor vurderes generelt ikke at påvirke den biologiske proces på renseanlæggene.

Den volumenmæssige belastning af erstatningsprodukter for fosfater består primært af zeolit (25%), natriumkarbonat (20%), natriumsilikat (8%) og natriumcitrat (7%). Af disse produkter vurderes zeolit at have den mest omsiggribende effekt på renseanlæggenes drift, idet zeolit vil akkumuleres i slammassen med op til 25-30% afhængigt af tilløbsbelastningen af zeolit. Dette vil reducere den organiske fraktion i slammet (VSS) og dermed modvirke den positive effekt af en formindsket simultanfældning som følge af mindre behov for fosforfjernelse.

Undersøgelser har vist, at slamafvandingsegenskaberne kan blive reduceret med 40% eller mere, hvilket vil forøge slamvoluminerne væsentligt medmindre metoder til en forbedret slamafvanding (teknologi/kemikalier) kan opveje dette fænomen. Denne problemstilling er imidlertid ret kompliceret og ikke særlig velbelyst i litteraturen. Problemet angående den nedsatte filtreringsevne af zeolitholdigt slam er påvist af flere, men der er ikke fundet artikler, som belyser, hvordan problemet evt. kan nedsættes ved tilsætning af polymerer i forbindelse med slambehandlingen. Udviklingen af polymerer der kan forbedre slamafvandingen har de sidste 10-20 år vist, at ændringen af slammets kemi vil føre til en væsentlig reduktion af slamvoluminerne, og det må formodes, at denne udvikling også vil komme zeolitholdigt slam til gode. Overordnet set vil reducerede slamfiltreringsegenskaber betyde, at

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[1] Oplysninger om anvendelsen af fosfor i tekstilvaskemidler og maskinopvaskemidler er indhentet i 2007. Ifølge SPT er andelen af fosfor i begge typer vaskemidler lavere i 2009.

slamvoluminerne, der skal bortkøres fra eller behandles på renseanlægget, vil forøges, men da der formentligt vil blive tilsat færre fældningskemikalier til fjernelse af fosfor vil dette problem blive reduceret i væsentligt grad – og muligvis slet ikke opstå.

Der var inden for dette projekts rammer ikke mulighed for at undersøge de faktiske forhold på renseanlæggene, og det vil sikkert også være vanskeligt at bestemme den reelle effekt på givne renseanlæg, idet problemet givetvis er afhængigt af mange faktorer såsom spildevandssammensætningen, zeolitbelastningen, vandets generelle hårdhed samt procesforholdene på renseanlægget (herunder fosforfjernelsen som nok vil være mindre på renseanlæg som modtager zeolitholdigt spildevand). Det kan være muligt at sammenligne renseanlæg, som er sammenlignelige mht. biologisk proces, belastning og slambehandling, men hvor det ene renseanlæg modtager zeolitholdigt spildevand, og det andet modtager fosfatholdigt spildevand. En sådan sammenligning kræver imidlertid, at en række renseanlæg med sådan en karakteristik kan findes, og at der er tilstrækkeligt med data til rådighed.

For at komme problemet til bunds vil det være mest relevant at gennemføre egentlige forsøg (lab./pilotskala) med både spildevandsbehandling og den efterfølgende slambehandling.

I øvrigt ses der ingen tegn på, at den biologiske proces på nogen måde vil blive inhiberet af de fosfatfrie vaskemidlers erstatningsstoffers tilstedeværelse i spildevandet.

Konklusioner

På baggrund af resultaterne af screeningen og risikovurderingen foretaget på erstatningsstoffer med den højeste risiko vil et forbud mod fosfat i tekstilvaskemidler ikke føre til toksiske effekter i vandmiljøet.

Overordnet set vurderes den resulterende effekt på de danske renseanlæg at være en reduktion i renseanlæggenes driftsomkostninger som følge af et reduceret kemikalieforbrug samt en formentligt uændret slamproduktion, såfremt det antages, at en betydelig reduktion af slamafvandingsegenskaberne ikke vil finde sted som følge af det forøgede zeolitindhold i slammassen. På trods af mulig reduktion i driftsomkostninger kan der blive behov for udgifter forbundet med procesomlægning samt til- eller ombygning af renseanlæg.

Summary and conclusions

A proposal on limitation on usage of phosphates in household detergents may be released by the EU Commission or proposed as part of the HELCOM Baltic Sea Action Plan. The purpose of this project is to carry out an environmental impact assessment of the potential substitutes for phosphates in laundry detergents and to assess the consequences on the wastewater treatment from the substitution of phosphate and the increased use of the alternative substances.

The project identifies substances for substitution of phosphate in laundry and automatic dishwashing detergents. The most important substitutes for phosphates in laundry detergents are zeolites, polycarboxylates, citrates and phosphonates. New alternatives as IminoDiSuccinate (IDS), Methyl Glycin Diacetic Acid (MGDA) and GLutamic acid Diacetic Acid (GLDA) are also introduced in builder systems today but to a smaller extend. Most important as alternatives to phosphates in automatic dishwashing products are citrates, silicates and carbonates.

An environmental assessment was carried out for the aquatic environment as a stepwise process. The environmental assessment did not include effects on the terrestrial environment. First an initial screening identified the substances with the highest hazard potential. The screening was based on typical concentration of the phosphate alternatives in laundry detergents and automatic dishwashing products. Parameters from the Detergent Ingredients Database list (DID list) from the European and Nordic ecolabels were used to calculate a risk index which indicates the environmental hazard potential of the substances. For the substances with the highest hazard potential, a determination of predicted environmental concentrations, PEC was carried out by use of two concepts, EUSES and ECO Lab modeling. Ecotoxicological data was found in available databases and the Predicted No Effect Concentrations ($PNEC_{aquatic}$) were derived according to the principles in the EU Technical Guidance Document for risk assessment (TGD). The risk quotients, RQ as the PEC/PNEC ratio were determined as the result of the environmental risk assessment for chronic as well as for acute exposure.

The screening identifies sodium silicate and zeolite as the substitutes for phosphate in laundry detergents with the highest environmental hazard potential. For automatic dishwashing products sodium silicate is the phosphate alternative with the highest hazard potential based on results of the screening.

An aquatic risk assessment was conducted for sodium silicate, zeolite, phosphonates and IDS (Iminodisuccinate) with focus on their use as substitutes for phosphates in laundry detergents. The risk quotient (RQ) calculated for chronic exposure and for acute exposure were all calculated to be below 1 indicating that use of the phosphate alternatives in laundry detergents is not expected to pose a risk to the aquatic environment.

The consequences on the wastewater treatment plant operation and performance of an expected change in the load of phosphorus and replacement with alternative substances were evaluated.

The calculation of the phosphorous load on Danish wastewater treatment plants was determined on the basis of estimations of household consumption of detergents in Denmark. When comparing this calculation of household consumption of detergents with that of the Danish EPA, a significantly larger amount of detergents was found (51,751 tonnes detergents/year as compared to 28,700 tonnes/year as assumed by the Danish EPA in 2001). When these figures are compared with those from Statistics Denmark, both estimates are much lower since the Statistics Denmark has estimated a household consumption of 78,364 tonnes/year. These differing figures indicate that the estimations of the actual consumption of detergents in Danish households are subject to significant uncertainty.

By introducing a phosphate ban of laundry and automatic dishwashing detergents (powder and tabs) in private households, the phosphate concentration level in municipal wastewater will be significantly reduced since. Presently 60-70% of washing detergents and 100% of automatic dishwashing detergents still contains phosphate[2]. Assuming that the Danish households consume 51.751 tonnes detergents/year it is estimated that the reduction in phosphate load to wastewater treatment plants could be as high as 46% - a reduction of 2,450 tonnes of phosphorus per year. The phosphorus concentration level in wastewater of 8.9 mg P/L is expected to be reduced to 4.8 mg P/L in average as a consequence of a full phosphate substitution in household detergents.

The impacts of this on the wastewater treatment plant operation is comprehensive since it probably will result in an almost complete diminishment of chemical precipitation processes, which today accounts for 30-40% of the total phosphorus removal and is responsible for a significant amount of the sludge production at Danish wastewater treatment plants. A significant saving of precipitation chemicals results in a reduction of the operation costs in the order of 50 mill. DKK per year. However, modifications of processes and alterations of buildings and other constructions at the wastewater treatment plant may be needed. The lower phosphorus concentration is in general not expected to affect the biological processes.

The volumetric load of alternative builder products to wastewater treatment plants will mainly constitute zeolite (25%), sodium carbonate (20%), sodium silicate (8%) and sodium citrate (7%). Zeolite is expected to have the most predominant impact on the wastewater treatment plant performance. Zeolite will accumulate in the sludge matrix with up to 25-30%, depending on the loading to the wastewater treatment plant. This will reduce the organic fraction of the sludge and counteract on the reduced chemical precipitation in the biological process. Investigations have shown that sludge dewatering can be reduced by at least 40%, which will increase the sludge volumes with the same amount unless methods to dewater sludge as efficiently as today are developed. However, this phenomenon is rather complicated and not very well documented in the literature. The reduced sludge dewatering of zeolite-containing sludge has been documented by several investigations, but none of

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[2] Information on the use of phosphate in detergents for laundry and automatic dish wash were collected during 2007. According to SPT the use of phosphate in both types of detergents are lower in 2009.

them have investigated how this phenomenon can be counteracted, e.g. by addition of sludge polymers in the sludge treatment operation. For the past 10-20 years, the development of sludge-dewatering polymers has shown that a change in the chemistry of sludge has a remarkable effect on the reduction of sludge volumes from wastewater treatment plants and it must be assumed that this development will also benefit zeolite-containing sludge. Reduced sludge-dewatering conditions will naturally lead to increased sludge volumes but since the addition of precipitation chemicals will be significantly reduced, this problem might never arise.

Within the framework of this project, it has not been possible to clarify the actual conditions at wastewater treatment plants receiving zeolite-containing wastewater. It is probably very difficult to determine the actual effect on the wastewater treatment plants since this effect most probably is determined by many factors like wastewater composition, the zeolite load, the alkalinity (hardness) of the water as well as the process conditions on the wastewater treatment plants. It might be possible to compare wastewater treatment plants that are comparable with respect to the biological process they perform, their load and the sludge treatment they conduct and one wastewater treatment plant receiving zeolite-containing wastewater (zeolite-containing detergents) and the other receiving wastewater without zeolite (phosphate-containing detergents). However, such a comparison requires a larger number of comparable wastewater treatment plants in order to be statistically relevant to evaluate.

In order to investigate the phenomenon thoroughly, it is recommended to conduct actual experiments under well-defined conditions (laboratory and pilot scale investigations under controlled conditions) including both wastewater and sludge treatment investigations.

There are no references indicating that phosphate-free detergents (zeolites) in any way inhibit the biological processes of the wastewater treatment plants.

Conclusions

Based on the results of the screening and the risk assessment of the substances with highest risk a ban of phosphate in laundry detergents will not lead to toxic effects in the aquatic environment.

Effects on Danish wastewater treatment plants from a ban of phosphate will most likely result the in lower operation costs in terms of less use of precipitation chemicals and a lower sludge production assuming that the resulting effect of sludge dewatering will not be seriously affected by the presence of zeolite. However expenses may be needed for modifications of processes and alterations of buildings and other constructions at the wastewater treatment plant.

1 Identification of substances for the substitution of phosphate

The identification of substances for the substitution of phosphate in detergents has been conducted as a dialog between DHI and the Association of Danish Cosmetics, Toiletries, Soap and Detergent Industries (SPT) and various representatives from the industry (2007). Focus has been on substances in laundry detergent and detergents for automatic dishwashing for consumer use.

Phosphate and the alternatives for phosphates are used as builders to enhance the surfactant effect in the detergents. The role of the builders is to lower the water hardness by scavenging the calcium and magnesium ions by adsorbing or chelating them.

The most important substitutes for phosphates in laundry detergents are zeolites and polycarboxylates. Others are phosphonates, carbonates and different carboxylates such as citrates and succinates. Citrates are used in certain products. The phosphonates have different properties in the laundry detergent and are normally used in very low concentrations as part of the builder system together with other complex binding substances. Sodium tartrate and sodium gluconate are only used very seldom and not considered as important substitute for phosphates. The zeolites are not used in liquid laundry products. For the liquid systems, the substitution of phosphate may take place by the use of e.g. IminoDiSuccinate (IDS). The IDS is a new chelating agent belonging to the aminocarboxylates.

Usage of NTA and EDTA has not been confirmed by the industry in the products used for the Danish market neither in consumer products nor in industrial products.

New environmental friendly builders are available today. The new alternatives are having a good or strong complex binding effect. They are all biological biodegradable and therefore considered as a good environmental alternative to phosphates. The most important is IminoDiSuccinate (IDS). Also Methyl Glycin Diacetic Acid (MGDA) and GLutamic acid Diacetic Acid (GLDA) are used in builder systems though it is in low amounts as the new substances are expensive alternatives to phosphates.

According to the industry, substitution of phosphates in the builder system in dishwashing products may lead to a product that is not as effective as the phosphate-containing product. The alternatives are not as good as phosphates to lower the hardness of the water. Alternatives to phosphates in automatic dishwashing products are a system consisting of citrates and silicates or carbonates. IDS may also be used as alternative to phosphates in automatic dishwashing systems. A prioritized list of alternatives for phosphates according to SPT and the industry is shown in Table 1-1.

Table 1-1 Gross list of identified substances for substitution of phosphate in laundry detergents and automatic dishwashing products

Substance Name
Zeolites
Polycarboxylates/Polyacrylates
Sodium citrate
Citric acid
Sodium carbonate
Sodium bicarbonate
Sodium silicate
Phosphonates
Sodium tartrate[3]
Sodium gluconate[3]
IDS (IminoDiSuccinate)[4]
MGDA (Methyl Glycin Diacetic Acid)[4]
GLDA (GLutamic acid Diacetic Acid)[4]
NTA (NitriloTriacetic Acid)[5]
EDTA (Ethylene Diamine Tetraacetic Acid)[5]

In a report prepared by the Swedish Chemical Agency (2006), substances for the substitution of phosphates are identified. In the report, zeolites are described as dominating alternatives for phosphate. Other alternatives are citrate, polyacrylates and to a lesser extend phosphonate and EDTA. For automatic dishwashing products, NTA is mentioned as an alternative.

Table 1-2 lists the substances which are potential candidates for the substitution of phosphates in laundry detergents and detergents for automatic dishwashing (powders and tabs) with the concentration given in percentage (w/w) in the final product. The concentrations are used to calculate a risk index (R) for the individual substances in the environmental assessment of the alternative substances for phosphates.

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[3] Not important alternative for phosphate

[4] New potential alternative for phosphate, not important today

[5] The potential as alternative is indicated by SPT, but not confirmed by the industry (2007)

Table 1-2 List of identified substances for substitution of phosphate in laundry detergents and automatic dishwashing products. The concentration in the products is given as the typical concentration based on average values (% w/w)

Substance name	Typical concentration in final product (% w/w)
Laundry detergents	
Zeolites	25
Polycarboxylates/Polyacrylates	1
Sodium citrate	7
Citric acid	2.5
Sodium carbonate	20
Sodium bicarbonate	30
Sodium silicate	8
Phosphonates	0.5
Sodium tartrate	2.5
Sodium gluconate	2.5
IDS (IminoDiSuccinate)	2.5
MGDA (Methyl Glycin Diacetic Acid)	1.0
GLDA (GLutamic acid Diacetic Acid)	2.5
NTA (NitriloTriacetic Acid)	-
EDTA (Ethylene Diamine Tetraacetic Acid)	-
Detergents for automatic dishwashing	
Sodium citrate	15
Citric acid	15
Sodium carbonate	15
Sodium bicarbonate	23
Sodium silicate	15

As background for the environmental assessment and the impact assessment on wastewater treatment plants recipes for prototypes of laundry detergents and tabs for automatic dishwashing has been set up. The prototypes are set up both for the builder system in phosphate-free system and phosphate-containing systems. An overview of the prototypes is shown in Appendix A as well as the approximations used as the background for the assessments.

2 Environmental assessment of substances for substitution of phosphate

The environmental assessment of the substances for substitution of phosphate in laundry detergents is carried out by a stepwise process consisting of an initial screening of the alternatives identifying the substances with the highest hazard potential, determination of predicted environmental concentrations, PEC and predicted no effects concentrations, PNEC and finally determination of risk quotients, RQ for substances identified in the screening assessment. In the derivation of RQ, the PEC is estimated by use of two concepts, EUSES and ECO lab modelling and the PNEC is calculated based on ecotoxicological studies and derived assessment factors for the individual substances.

The risk assessment is limited to cover the aquatic environment as no effect to sediment or soil organisms are known for the phosphate substitutes.

2.1 Screening for potential environmental hazard

An initial screening of the possible candidates for the substitution of phosphate is conducted. The aim of the screening is to identify substances with the highest environmental hazard potential based on the calculated risk index (R). The screening involves an initial calculation of how much of the individual substances will enter and leave the sewage treatment plant. The amount entering (IN) is dependent on the dosage of the product (e.g. weight of laundry detergent per wash) and the percentage of the substance in the product. In general, the amount leaving the sewage system (OUT) will depend on the removal taking place in the sewage treatment plant e.g. biological degradation, evaporation, sorption etc. In order to ease the screening only removal from biological degradation in the wastewater treatment plant is considered here and a degradation factor describing the biodegradability is used to estimate the effluent from the wastewater treatment plant.

The risk index is calculated based on the amount leaving the sewage system and a toxicity factor, which in the screening will be derived from the Detergent Ingredients Database list (DID-list; www.ecolabel.dk). In the calculations of the PNEC values to be used in the environmental risk assessment ecotoxicological data from existing databases (US-EPA, IUCLID and QSAR calculations) as well as an environmental risk assessment previously conducted by DHI (Danish EPA, 2001) will be used in order to use data for the exact substances where possible.

2.1.1 Degradation factor

The degradation factor for each substance is set according to the current criteria listed for the “EU-Flower” and the “Nordic Swan” ecolabel (www.ecolabel.dk). According to the ecolabel criteria, the degradation factor is 0.05 if a compound is readily biodegradable, 0.5 if the compound is inherently biodegradable and 1 if a substance is persistent.

Table 2-1 Degradation factors (DF)

Substance name	DF
Zeolite 1318-02-1	1¹⁾
Polycarboxylate	1¹⁾
Sodium citrate (Disodium citrate/Trisodium citrate) 144-33-2/ 68-04-2	0.05²⁾
Citric acid 77-92-9	0.05¹⁾
Sodium carbonate/bicarbonate 497-19-8 / 144-55-8	0,15¹⁾
Sodium silicate 1344-09-8	1⁴⁾
Phosphonate 6419-19-8 15827-60-8 2809-21-4	1¹⁾
Sodium tartrate	0,5⁴⁾
Sodium gluconate 527-07-1	0.05¹⁾
IDS (Iminodisuccinate) 144538-83-0	0.05¹⁾
MGDA (Methyl glycin diacetic acid)	0.05¹⁾
GLDA (GLutamic acid Diacetic Acid) (L-form)	0.05³⁾

1) DID list, 2007
2) Danish EPA, 2001
3) Dissolvin, 2007
4) Based on evaluation of chemical structure

Two CAS numbers are listed for sodium citrate, where no data was found for the monoform and therefore data for disodium and trisodium citrate are presented. The CAS numbers presented for phosphonate are taken from the Swedish report “Fosfater i tvätt- och rengöringsmedel” (Swedish Chemicals Agency, 2006) as the representatives of phosphonates for this group.

The degradation factor for GLDA is for the L isomer only as according to the information derived from Dissolvin (2007) only this form and not the D-form is biodegradable.

2.1.2 Release from wastewater treatment plant

In order to evaluate the risk index of the use of a product an estimation of the amount of the substance in the effluent of the sewage treatment plant is done. It is assumed that the dosage (X) is 70 g per wash of laundry and the dosage is 22 g per automatic dish wash (See Appendix A). The amount of a substance entering the sewage treatment plant per wash can be calculated as followed:

$$IN\ (g) = X\ (g) \times \text{conc. of substance in the detergent (\%)}$$

And the amount leaving the sewage treatment plant per wash can be calculated as followed:

*OUT (g) = X (g) × conc. of substance in the detergent (%)*DF*

Where
IN is the amount of the substance entering the sewage system per wash
OUT is amount of the substance leaving the sewage system per wash
X is the dosage of detergents for laundry or automatic dishwashing
DF is the Degradation Factor.

Using the typical concentration (%) listed in Table 1-2, the results listed in Table 2-2 are obtained.

Table 2-2 Calculated amounts (g) entering (IN) and leaving (OUT) the sewage treatment plant

Substance name	IN (g)	OUT (g)
Laundry detergents		
Zeolite	17.5	17.5
Polycarboxylates	0.7	0.7
Sodium citrate	4.9	0.25
Citric acid	1.8	0.1
Sodium carbonate	14.0	2.1
Sodium bicarbonate	21.0	3.2
Sodium silicate	5.6	5.6
Phosphonates	0.35	0.35
Sodium tartrate	1,75	0,88
Sodium gluconate	1.75	0.09
MGDA (Methyl glycin diacetic acid)	0.7	0.04
IDS (Iminodisuccinate)	1.75	0.09
GLDA (GLutamic acid Diacetic Acid) (L-form)	1.75	0.09
Detergents for automatic dishwashing		
Sodium carbonate	3.3	0.5
Sodium bicarbonate	5.1	0.77
Sodium silicate	3.3	3.3
Citric acid	3.3	0.17
Sodium citrate	3.3	0.17

2.1.3 Risk index for the aquatic environment

In order to evaluate which substances are associated with the highest environmental hazard potential when substituting phosphate, a risk index (R) is calculated.

The risk index (R) is given as: *R = OUT/TF*

Where
OUT is the of the substance leaving the sewage system per wash (Table 2-2)
TF (Toxicity Factor) is derived based on the lowest NOEC value (or EC50-value from long term test) for the substance (Table 2-3) (DID-list, 2007).

The TF is taken from the DID-list in this pre screening as mentioned previously (Section 2.1).

Substances with the highest R-value are considered to have the highest hazard potential for adverse effects when entering the aquatic environment through a sewage treatment plant.

Table 2-3 Toxicity Factor (TF) and risk index (R) for phosphate substitutes

Substance name	TF[1)]	R
Laundry detergents		
Zeolite	3.5	5.00
Polycarboxylates	10.6	0.07
Sodium citrate*	1.6	0.16
Citric acid	1.6	0.06
Sodium carbonate**	0.25	8.40
Sodium bicarbonate**	0.25	12.8
Sodium silicate***	0.25	22.4
Phosphonates	0.5	0.70
Sodium tartrate	No data	-
Sodium gluconate	1	0.09
MGDA (Methyl glycin diacetic acid)****	0.334	0.12
IDS (Iminodisuccinate)	0.17	0.53
GLDA (GLutamic acid Diacetic Acid) (L-form)	No data	-
Detergents for automatic dishwashing		
Sodium carbonate**	0.25	2.00
Sodium bicarbonate**	0.25	3.08
Sodium silicate***	0.25	13.2
Citric acid	1.6	0.11
Sodium citrate*	1.6	0.11

1) DID list, 2007
* TF for citrate
** TF for carbonates
*** TF for silicates
**** TF for trisodium methylglycin diacetate

No data were available for GLDA and therefore no R is calculated.

2.2 Substances with high environmental hazard potential

Table 2-4 lists the substitutes for phosphate after their potential to cause adverse effects in the aquatic environment as indicated by use of the values in the DID-list. According to the results of the screening in this study the substances with the highest risk index (R) are sodium silicate, sodium bicarbonate, sodium carbonate and zeolite for the substitution of phosphate in laundry detergents. For automatic dishwashing detergents, sodium silicate, sodium bicarbonate and sodium carbonate are the substances with the highest risk index based on the results of the screening. The reason for the high R value is a combination of a relatively low TF and that these substances are used in a higher percentage (see Table 1-2) in the products. The screening of the hazard potential of the substances is based on simple indicators for degradation and aquatic toxicity derived from the DID-list. The screening approach implies that a high value of the risk index (R) does not confirm that the use of the substance in household detergents presents a risk to the aquatic environment, but merely that further assessments are necessary.

The screening points to sodium carbonate and sodium bicarbonate among the substitutes with the highest hazard potential. Carbonate and bicarbonate are prevalent in all natural aqueous systems where they are in equilibrium together. Under strongly alkaline conditions carbonate is predominant, whereas bicarbonate prevails under weakly alkaline conditions. Reservations may be taken to the results from the screening applied here due to the facts mentioned and that the buffer capacity of the receiving aqueous system was not accounted for. Carbonate will be neutralised in wastewater treatment plants and sodium itself has a low toxicity (HERA, 2009).

The following sections 2.3-2.5 include a detailed aquatic risk assessment of the substances characterised by high risk indexes in the screening assessment. The risk assessment will not be done on sodium bicarbonate and sodium carbonate due to the reasons mentioned above.

Table 2-4 Substitutes for phosphate according to their degree of risk (R)

Substance name	R
Sodium silicate	22.4
Sodium bicarbonate	12.8
Sodium carbonate	8.40
Zeolite	5.00
Phosphonates	0.70
IDS (Iminodisuccinate)	0.53
Sodium citrate	0.16
MGDA (Methyl glycin diacetic acid)	0.12
Sodium gluconate	0.09
Polycarboxylates	0.07
Citric acid	0.06
Sodium tartrate	-
GLDA (GLutamic acid Diacetic Acid) (L-form)	-
Detergent for automatic dishwashing	
Sodium silicate	13.2
Sodium bicarbonate	3.08
Sodium carbonate	2.00
Citric acid	0.11
Sodium citrate	0.11

The Swedish report “Fosfater i tvätt- och rengöringsmedel” (Swedish Chemicals Agency, 2006) describes the zeolites as having low toxicity towards aquatic organisms (only minor effects on algae are observed) and it is mentioned that there are no signs of risks to human health (CMR). According to the report, and numerous other references, citrates are easily biodegradable in the environment, they are not bioaccumulative and they are non-toxic to aquatic organisms. Likewise, polycarboxylates have a low toxicity and are not bioaccumulative because of their large molecular weight. Phosphonates are described as having a low biodegradability and as non-bioaccumulative because they are very water soluble. Some phosphonates are reported to have a high toxicity and care should be taken, keeping in mind the low biodegradability.

In this study, an aquatic risk assessment will be conducted for zeolite, sodium silicate, phosphonates and IDS with focus on their use as substitute for phosphates in laundry detergents.

2.3 Derivation of PNEC

The information on the intrinsic ecotoxicological properties of the substances listed in Appendix B was obtained from a review of existing databases (US-EPA, IUCLID and QSAR calculations) as well as an environmental risk assessment for several of the above mentioned substances which was previously conducted by DHI (Danish EPA, 2001). The data on ecotoxicological properties are used for the exact substances where identified by the CAS numbers. For IDS ecotoxicological data were obtained from data on the commercial raw material Baypure^{TM} CX 100 solid consisting of more than 65 % by weight of IDS.

Values for the aquatic toxicity of substances listed in the Appendix B are given by the results from the studies with the highest toxicity, i.e. studies which have resulted in a low NOEC/EC_{50}/LC_{50}, in order to calculate a Predicted No Effect Concentration ($PNEC_{aquatic}$). These values are highlighted in Appendix B.

The derivation of a Predicted No Effect Concentration ($PNEC_{aquatic}$) for a substance involves the application of an assessment factor (AF). The assessment factor expresses the difference between the effect concentration values derived from laboratory tests and the derivation of the $PNEC_{aquatic}$. The size of the AF depends on the number relevant studies, the number of trophic levels and taxonomic groups covered by the data, and the availability of data from long-term chronic tests. AFs are applied according to the principles listed in the Technical Guidance Document (TGD, 2003) and listed in Table 2-5 together with the derived $PNEC_{aquatic}$. For Sodium silicate ecotoxicological data for fish and crustacean show a low toxicity (EC_{50}/LC_{50}/NOEC >100 mg/L) and we would expect the toxicity for algae to be low as well. Therefore, an assessment factor of 1,000 is applied for this compound. An assessment factor of 100 was applied on the long term NOEC for algae, which is considered to be the most sensitive organism.

The $PNEC_{aquatic}$ in Table 2-5 is representing the chronic PNEC. In general, it may be assumed that the acute PNEC is 10 times higher than the chronic PNEC.

Table 2-5 Calculated PNEC for the aquatic environment

Substance	Assessment Factor (AF)	$PNEC_{aquatic}$ (mg/L)
Sodium silicate 6834-92-0	1,000	0.216
Zeolite 1318-02-1	10	7
Phosphonates 2809-21-4	100	0.03
IDS (Iminodisuccinate) 144538-83-0	10	2.28

2.4 Derivation of PEC

For the derivation of a Predicted Environmental Concentration (PEC) for the identified substances with highest risk two methods where applied: EUSES and ECO Lab.

2.4.1 Use of EUSES

EUSES is a decision-support instrument, which enables a rapid and efficient assessment of the general risks posed by substances to man and the environment. The EUSES estimation is based on the principles described in the TGD (2003). In this project, EUSES was used to estimate the environmental concentrations of the four phosphate substitutes. For the estimations of PEC, the EU TGD 2003 Risk Assessment Spreadsheet Model (2007) was used. The spreadsheet model was chosen in order to ease the estimations of the PEC values, as the properties of the substances identified in this project allowed the spreadsheet to be used. The two inorganic substances and the phosphonates are considered as conservative substances with no evaporation, absorption or degradation in the sewage treatment plant. Hence, the EUSES calculations represent a worst-case scenario with no treatment. Data on (1-hydroxyethylidene) bis phosphonic acid (CAS nr. 2809-21-4) are used for the estimation of PEC on phospohonates. For IDS the biodegradability of the substance is taken into account in the estimation of PEC.

For each of the four substances, data on physical-chemical substance properties, degradation and transformation rates and emissions are put into the risk assessment spreadsheet.

In order to estimate the local emission to wastewater, the number of households in Denmark has to be taken into account. Information of the number of households given in Table 2-6 is collected from Statistics Denmark (2007).

Table 2-6 Information on numbers of households in Denmark

Number of households in DK	2,532,000
Number of households with one person	1,094,000
Number of households with more than one person	1,438,000

To estimate the emission to the wastewater, it is assumed that 90% of the waste water from all households is discharged to the sewage system. It is assumed that single families are doing 150 laundries per year and other families are doing 400 laundries per year. The approximations listed in Appendix A regarding use of phosphate-free laundry detergents and the typical concentrations listed in Table 1-2 are used to calculate the emission of each substance. Table 2-7 shows the data used in the EUSES estimation.

Table 2-7 Overview of data used in the EUSES estimation

	Water solubility (g/L)	Conc. in laundry detergent (% by weight)	Total emission to wastewater treatment plant[1]	
			(t/year)	(Kg/d)
Sodium silicate	200	8	3.7	10
Zeolite	0	25	12	32
Phosphonates	690	0.5	0.23	0.64
IDS (Iminodisuccinate)	25	2.5	1.2	3.2

1) Total emission of laundry detergents to wastewater in Denmark was estimated to 46,576 t/year

The input values used in the calculations and the output from the calculation are shown in Appendix D. The PEC-values are estimated for the local surface water and the local marine water (Table 2-8). The maximum and the average value are the same using the EUSES model for conservative substances.

Table 2-8 Predicted Environmental Concentration from the EUSES estimation

	$PEC_{local.water}$ (mg/L)	$PEC_{local.water,marine}$ (mg/L)
Sodium silicate	0.51	0.051
Zeolite	0.5	0.05
Phosphonates	0.03	0.003
IDS (Iminodisuccinate)	0.02	0.002

2.4.2 Emission/inventory and ECO Lab model

In the ECO Lab modelling, Little Belt was chosen as the Danish surface water scenario. Appendix C describes the background for the ECO Lab model in detail. Results are given in Table 2-9.

Table 2-9 Calculated PEC value given as maximum and average values and presented as 90th percentile, when the concentration in the outlet from the sewage treatment plant is 1 mg/L

Station	Max	Average	Unit
PEC90th	0.1017	0.01885	mg/L

PEC90th : the 90th percentile

It is assumed that a person uses 200 L of water each day. And that a household of 4 persons has in average 1 wash per day (i.e. 0.25 wash per person per day). Again, the dosage for laundry detergent (X) is assumed to be 70 g/wash.

PEC_{inlet} = ***(X (g)*** × ***conc. of substance in the detergent (%)*** × ***0.25) / 200 L/day***

$PEC_{outlet} = PEC_{inlet} \times (DF)$ ***(DF taken from*** Table 2-1)

$PEC_{average} = PEC_{outlet} \times 90^{th}PEC_{average} / 1\ mg/L$

$PEC_{max} = PEC_{outlet} \times 90^{th}\ PEC_{max} / 1\ mg/L$

Where

PEC_{inlet}	is the Predicted environmental concentration in the inlet
PEC_{outlet}	is the Predicted environmental concentration in the outlet of the sewage treatment system
$PEC_{average}$	is the average Predicted environmental concentration close to the outlet of a STP
PEC_{max}	is the maximum Predicted environmental concentration close to the outlet of a STP

Example for Zeolite (laundry detergent)

PEC_{inlet} = (70 g/wash × 25 % × 0.25 wash/day)/200 L/day = 0.022 g/L = 22 mg/L

PEC_{outlet} = 0.022 g/L × 1 = 0.022 g/L = 22 mg/L

PEC_{max} = 0.1017 × 22 mg/L = ***2.2 mg/L***

$PEC_{average}$ = 0.01885 × 22 mg/L = ***0.41 mg/L***

Table 2-10 Predicted Environmental Concentration from the ECO Lab modelling

Substance name	$PEC_{average}$	PEC_{max}
Sodium silicate	0.13	0.71
Zeolite	0.41	2.2
Phosphonates	0.0082	0.044
IDS (Iminodisuccinate)	0.0021	0.011

2.5 Aquatic risk assessment

In order to evaluate the risk involved with the usage of the high risk substances, a Risk Quotient (RQ) is calculated as the ratio

RQ = PEC/PNEC

The estimation of RQ based on the PEC values obtained by use of the EUSES is shown in Table 2-11. The $PEC_{local.water}$ is used for estimation of the RQ_{acute} and the $RQ_{chronic}$ is derived by the $PEC_{local.water,marine}$.

Table 2-11 Calculated Risk Quotient (R) based on PEC estimated by use of EUSES

Substance name	$RQ_{chronic}$	RQ_{acute}
Sodium silicate	0.24	0.24
Zeolite	0.007	0.007
Phosphonates	0.1	0.1
IDS (Iminodisuccinate)	0.001	0.001

The estimation of RQ based on the ECO Lab modelling is shown in Table 2-10. $PEC_{average}$ is used to evaluate the RQ of chronic exposure and the PEC_{max} is used to evaluate the RQ of acute exposure. We earlier derived a $PNEC_{aquatic}$ which in this case is representing $PNEC_{chronic}$ (Table 2-5) and it is assumed that the $PNEC_{acute}$ is 10 times higher than the $PNEC_{chronic}$ i.e. values in Table 2-5 are multiplied by 10 in order to calculate RQ_{acute}.

Table 2-12 Calculated Risk Quotient (R) based on PEC derived from the ECO Lab modelling

Substance name	$RQ_{chronic}$	RQ_{acute}
Sodium silicate	0.611	0.330
Zeolite	0.059	0.032
Phosphonates	0.22	0.15
IDS (Iminodisuccinate)	0.001	0.0005

According to the TGD, if the RQ is below 1, the risk to the environmental compartment is considered to be acceptable. An RQ above 1 indicates a potential risk. Following this, none of the phosphate substitutes pose a risk to the aquatic environment since all calculated RQ values are below 1.

2.6 Conclusions

The environmental risk assessment was carried out for the substances with the highest risk index derived in the screening assessment.The results of the risk assessment indicate that substitution of phosphate in household detergents will lead to environmental concentrations of the substitutes which are below the no observed effect concentrations for the substances. On this basis, it is unlikely that a ban of phosphate in laundry detergents will lead to toxic effects in the aquatic environment. The screening and the risk assessment is based on prototypes for phosphate-free detergents for laundry which are typical for the use today. However, this may be changed by a ban of phosphate, which potentially may lower the price on the new alternative substitutes as IDS, GLDA and MGDA. The substitutes are all considered as easily biodegradable and therefore anticipated to be biodegraded during treatment in the wastewater treatment plants.

3 Impact assessment of substitution of phosphates on wastewater treatment plants

By substituting phosphorus in laundry detergents with phosphate-free builders, the phosphorus inlet concentration is expected to be significantly reduced and concentrations of replacement builders will increase. According to SPT 60-70% of the laundry detergents and 100% of automatic dishwashing detergents today contains phosphate, which means that a full substitution of phosphate with alternative complex building chemicals will result in significant increased load of these substances[6].

In this chapter, the expected load changes of phosphorus and alternative replacement substances will be determined and the effects on the wastewater treatment plant operation and performance will be discussed.

3.1 Compositions, assumptions and approximations

3.1.1 Composition of phosphate-containing and phosphate-free detergent builder systems

According to SPT phosphate-containing laundry detergents (powder) constitutes 60-70% of the total market volume in Denmark while all detergent products for automatic dishwashing detergents (washing tabs and powder) contain phosphates today. While the builder system in laundry powder detergents and automatic dishwashing detergents that contain phosphate is quite similar, the composition of phosphate-free detergents in laundry powder and automatic dishwashing detergents is more different. See Appendix A for prototypes of phosphate-free and phosphate-containing laundry detergents and products for automatic dishwashing.

Most importantly, phosphate-free laundry powder detergents are mainly built on inorganic zeolite while the automatic dishwashing phosphate-free detergents are built on organic acids/salts and inorganic silicates and carbon. The content of the inorganic mineral zeolite in phosphate-free washing powder is so significant that it will have an impact on the wastewater composition at the inlet of wastewater treatment plants (see Section 3.4). Phosphorus discharge from phosphate-containing ***laundry detergents*** can be estimating assuming a certain unit consumption of detergents (laundry powder) from each of the 2,532,000 households in Denmark (Statistics Denmark, 2007). Based on Statistics Denmark (2007) 1,094,000 persons are living alone in Denmark and if it is assumed that they perform 150 machine washes per year using 70 gram of washing powder per wash they will

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[6] Information on the use of phosphate in detergents for laundry and automatic dish wash were collected during 2007. According to SPT the use of phosphate in both types of detergents are lower in 2009, hence the consequences from a ban of phosphate will be less significant than assumed based on the 2007 numbers.

consume 11,487 tonnes of washing powder per year. Accordingly 1,438,000 families was registered in Denmark in 2006 and assuming that they perform 400 machine washes per year families in Denmark would consume 40,264 tonnes of washing powder per year. This results in a total consumption of ***51,751 tonnes washing powder per year***. This amount is higher than estimated in (Danish EPA, 2001) (28,700 tonnes/year) but lower than given in (Statistics Denmark, 2006) (78,364 tonnes/year).

The amount of phosphorus in laundry powder detergents is calculated based on the assumption that 90% of the detergents discharged by private households in Denmark reach the wastewater treatment plants, that 65% of the detergents contain phosphorus and that the weight percentage of phosphorus in washing powder is 5% (based on 25% P in phosphate). This results in a total phosphorus discharge from laundry powder detergents on 1,514 tonnes P/year.

Phosphorus discharge from phosphate-containing ***automatic dishwashing detergents*** has been estimating assuming a certain unit consumption of detergents (automatic dishwashing powder) from each of the 1,438,000 families in Denmark (Statistics Denmark, 2007). It is estimated that the 1,438,000 families perform 300 machine washes per year using 22 gram of automatic dishwashing powder per wash. It is assumed that the 1,094,000 single living persons do not use automatic dishwashing machines in their home. This results in a total consumption of ***9,491 tonnes automatic dishwashing powder per year***. This amount is also higher than estimated in (Danish EPA, 2001) (3,800 tonnes/year) but lower than given in (Statistics Denmark, 2006) (15,005 tonnes/year). The amount of phosphorus in automatic dishwashing powder detergents is calculated based on the assumption that 90% of the detergents reach the wastewater treatment plants, that 100% of the detergents contain phosphorus and that the weight percentage of phosphorus in washing powder is 11% (based on 25% P in phosphate). This results in a total phosphorus discharge from automatic dishwashing detergents on 960 tonnes P/year.

3.1.2 Phosphorus loads to wastewater treatment plants

According to Danish EPA (2004) Denmark has 1,193 municipal wastewater treatment plants with a capacity higher than 30 PE (2004). Most part of the wastewater (90%) is treated at 263 larger wastewater treatment plants that receive approximately 600 mill. m^3/year in total. The average inlet concentration of phosphorus to the larger wastewater treatment plants can based on this be calculated to 8.9 mg P/L, which results in a total phosphorus load to the wastewater treatment plant on 5,350 tonnes P/year (Danish EPA, 2004).

The phosphorus load to Danish wastewater treatment plants has been reduced significantly over the last 10-20 years. At Lynetten wastewater treatment plant, the phosphorus load has been reduced from 1,100 tonnes P in 1988 to 750 tonnes P in 1995. In 2006, Lynetten wastewater treatment plant received 509 tonnes/year (Lynetten, 2006), which resulted in an average phosphorus inlet concentration on 7.8 mg P/L. A major reason for the reduction of phosphorus load is partly believed to be caused by a reduced use of phosphorus-containing laundry detergents in private households and reduced industrial activity in the catchment area of Lynetten.

In Table 3-1, the major phosphorus load sources to the 263 largest wastewater treatment plants are listed. The major phosphorus sources come from human excretion (urine and faeces), detergents (laundry and automatic dishwashing) and other sources (other household load institutional and industrial sources).

Assuming that the population connected to the wastewater treatment plants excretes 0.5 kg P/year (Jönsson ***et. al***, 2005) and that 80% of the total phosphorus generation of the human discharge reaches the wastewater treatment plant this will result in a phosphorus load to the wastewater treatment plants on 1,940 tonnes P/year or 36% of the total phosphorus load to the wastewater treatment plants.

The amount of phosphorus originating from household detergents (laundry and automatic dishwashing was estimated to 2,475 tonnes P/year which constitutes 46% of the total phosphorus load today.

The remaining amount of phosphorus 935 tonnes P/year (18%) is assumed to originate from industrial sources (phosphorus discharged after internal pre-treatment) and from institutions other than human excretion.

Table 3-1 Phosphorus load to the 263 largest wastewater treatment plants in Denmark

Pollution source	Discharge	Unit
Human excretion	1,940 1)	Tonnes P/year
Phosphorus-containing laundry detergents	1,514 2)	Tonnes P/year
Phosphorus-containing automatic dishwashing detergents	961 3)	Tonnes P/year
Other sources	935	Tonnes P/year
Total phosphorus load to wastewater treatment plants	5,350 4)	Tonnes P/year

1) Assuming 80% discharge of total load from human phosphorus excretion will reach the wastewater treatment plants
2) Assuming 51,751 tonnes laundry detergents is discharged to the sewer system (65% phosphate-containing detergents) with a phosphorus (P) weight percent on 5 g/kg detergent
3) Assuming 9,491 tonnes automatic dishwashing detergents is discharged to the sewer system (100% phosphate-containing detergents) with a phosphorus (P) weight percent on 11 g/kg detergent
4) Phosphorus inlet load to the 263 largest wastewater treatment plants in Denmark, 2004 (Danish EPA, 2004)

3.2 Expected change in loads to wastewater treatment plants of substances originating from laundry and automatic dishwashing detergents

3.2.1 Change in phosphorus load to wastewater treatment plants

Assuming a total ban of phosphorus containing detergents for laundry and automatic dishwashing will be adopted, this will have a great impact on the phosphorus load to wastewater plant in Denmark. Assuming the load estimations of phosphorus to Danish wastewater treatment plant will be reduced with 2,475 tonnes P/year, the total load reduction of phosphorus will change from 5,350 tonnes P/year to 2,875 tonnes P/year. ***This will reduce the***

average inlet concentration of phosphorus from 8.9 mg P/L to 4.8 mg P/L (calculations based on 2004 data, adapted from Danish EPA (2004)).

3.2.2 Change in phosphate-free detergent load to wastewater treatment plants

Zeolites are volumetrically the most predominant chemical in phosphate-free detergent builder products. Furthermore, zeolites (zeolite A) are insoluble inorganic hydrated aluminosilicates ($Na_{12}(AlO_2)_{12}(SiO_2)_{12}\cdot 27H_2O$ that interacts and becomes a part of the biological sludge at wastewater treatment plants. Consequently, zeolite is the most relevant ingredient to focus on when determining load and impact of phosphate-free detergents on wastewater treatment plant performance and operation (Piirtola ***et al.***, 1998).

No records have been found on the presence of zeolite mineral in inlet wastewater to Danish wastewater treatment plants but if it is assumed that 35% of all washing powder detergents presently contain zeolite a total discharge on 4,075 tonnes zeolite to the wastewater treatment plants must presently be expected, which equals to an average inlet concentration on 6.8 mg zeolite/L. Assuming that phosphate-containing detergents will be replaced 100% with zeolite-containing builder products, a total load on 11,600 tonnes of zeolite will be discharged to municipal wastewater plants, which will increase the inlet concentration of zeolite to 19.3 mg/L. These numbers are in good correlation with Hopping (1978), Maki (1978) and Morse ***et al.*** (1994) who reported zeolite inlet concentrations in the range 10-30 mg/L. However, the inlet concentration of zeolite is very much depending on the hardness of groundwater, which is reflected by Fischer ***et al.*** (1978) who determined zeolite concentrations up to 60 mg/L in hard water areas of Germany.

3.3 Effects on the wastewater treatment plant operation as a result of reduced phosphorus load

3.3.1 Phosphorus removal in biological and chemical wastewater treatment processes

Today phosphorus is being removed efficiently at most Danish wastewater treatment plant by a combination of biological phosphorus removal and chemical precipitation of phosphorus. The biological processes require phosphorus for bacterial growth of heterotrophic as well as autotrophic bacteria. Since heterotrophic processes are the most predominant in terms of concentration and growth rate of biomass, the phosphorus requirement is normally calculated for this group of bacteria. According to Henze ***et. al*** (2000) the phosphorus requirement constitutes 1.5% of the sludge production, which normally account for 1/3 of the total phosphorus removal in municipal wastewater treatment plants (Gert Petersen, 2007). E.g. for removal of 500 mg COD/L the phosphorus requirement for the biological heterotrophic growth process would be 3.4 mg P/L for a normally observed yield of the process on 0.45 kg COD_B/kg COD_S.

Phosphorus is also being removed in the so-called Bio-P process where a special group of bacteria (mainly Acinetobacter) are able to accumulate a higher amount of phosphorus as storage products internally. This process is becoming more and more attractive in Denmark as a “green” alternative to traditional precipitation with chemicals since the additional phosphorus accumulation is removed with the excess sludge production without using chemicals. It is estimated that 30-40% of the total phosphorus removal in

Denmark today takes place as a result of the Bio-P process (Gert Petersen, 2007).

Chemical precipitation with ferrous or aluminium metal salts is the most traditional and widely used method of removing phosphorus in wastewater treatment processes. The advantage of using these metal salts for phosphorus removal is that the phosphorus removal efficiency can be controlled quite accurate and the effluent concentration of soluble phosphorus can be reduced to almost zero. The efficiency of the chemical phosphorus removal process is determined by the molar ratio between phosphorus and the metal salt. Normally a molar ratio of 1.0 mole Me/mole P is necessary to reduce the effluent phosphorus to 1.5 mg TP/L but in order to reduce tax payment of phosphorus discharge most Danish wastewater treatment plants try to obtain a phosphorus concentration below 0.5 mg P/L in the effluent, which requires a molar ratio of 1.5 mole Me/mole P. The result of the increased molar ratio is an increase in the sludge production on 50% (chemical sludge).

3.3.2 Phosphorus shortage for the biological processes

It is evident that a reduction of the phosphorus load will have a great impact on how wastewater treatment plants will be operated in the future. In case that a total ban of using phosphorus detergents for washing and automatic dishwashing in private households will be determined, the reduction of the phosphorus load to wastewater treatment plants will almost be reduced to half (46%), which means that most of the phosphorus can be removed biological and chemical sludge production will be minimized significantly. In fact, phosphorus shortage could be causing problems to some wastewater treatment plants that presently have low phosphorus concentrations in the inlet compared to the COD inlet concentration and as a result of that phosphorus has to be added to the biological processes on these wastewater treatment plants.

3.3.3 Sludge composition and production

A major benefit of a reduced precipitation with chemicals is the reduction in the chemical sludge production at the wastewater treatment plants. As a rule of thump removal of 1 kg phosphorus results in production of 15 kg suspended solids with a molar ratio between metal and phosphorus on 1.5 (Gert Petersen, 2007). Assuming 30% of all phosphorus is being removed chemically the potential reduction of chemical sludge production will be approximately 24,000 tonnes of sludge per year, which is about ¼ of the total sludge production in Denmark. However, the net reduction in sludge production will be much less because the substituted chemical in detergents (primarily zeolites) will contribute to the sludge production (Section 3.4.1).

3.3.4 Chemical savings

Another significant effect of a diminished chemical precipitation is the reduced use of chemical addition in the wastewater treatment plant. It is estimated that 40,000-50,000 tonnes precipitation chemical solution (iron chloride, iron sulphate and aluminium chloride primarily) can be saved as a result of the significantly reduced precipitation with chemicals, which will reduce the operation costs of Danish wastewater treatment plants in the order of 50 mill. DKK per year. Even though the need for phosphorus precipitation in theory can be prevented, chemical precipitation cannot be avoided in practice when the effluent concentration of soluble phosphorus should be treated down to very low concentrations (below 0.5 mg $P_{soluble}$/L). The chemical consumption will however be much lower because of the much lower phosphorus amounts that needs to be removed.

3.3.5 Increased volatile fatty acids (VFA) for denitrification

Biological phosphorus removal (Bio-P) will be reduced in case the full reduction of the phosphorus load will take place (46% reduction in the phosphorus load). This will reduce the need and efficiency of the Bio-P process since the phosphorus concentration level in the wastewater will be much lower. As the Bio-P process consumes large amount of VFA, the VFA consumption will be reduced, which can benefit the denitrification process. Hence, the nitrogen removal that consumes easily degradable organic matter will potentially be improved.

3.4 Expected effects on the wastewater treatment plant operation as a result of using phosphate-free detergents in private households

Substitution of phosphate builders with alternative builder products will result in a change in the sludge composition and behaviour on the wastewater treatment plants. The volumetric load of alternative builder products to wastewater treatment plants will mainly constitute zeolite (25%), sodium carbonate (20%), sodium silicate (8%) and sodium citrate (7%) and as mentioned earlier zeolite is expected to have the most predominant impact on the wastewater treatment plant performance. In the following focus is on the expected effects caused by a higher zeolite concentration in the incoming wastewater to the wastewater treatment plants.

3.4.1 Increased content of zeolite in the sludge composition

Zeolite will as an inert particulate organic compound accumulate in the biological sludge and displace a part of the organic fraction of the sludge. The actual build-up of zeolites depends on the specific plant operation – i.e. the mixed liqueur suspended sludge concentration (MLSS), the load of zeolites and the sludge production. Hence, it is difficult to state precisely how big a part of the organic sludge fraction the inorganic zeolites will drive out. Piirtola ***et al.*** (1998) reported an increase in sludge suspended solids of up to 25-30% in pilot tests where zeolite was added in concentrations that reflect the expected concentration increase of zeolite when substituted with phosphate builders in detergents. The result of this is that the MLSS concentration in the aeration tanks must be increased in order to avoid loss of nitrification at the plants. For wastewater treatment plants operated with simultaneously phosphorus precipitation, i.e. addition of precipitation chemicals directly in the MLSS, there might be status quo or even a reduction in the inorganic fraction of the sludge, which means that these wastewater treatment plants could be run with a lower MLSS set point in the aeration tank.

3.4.2 Effects on biological processes

Several of studies have been investigating the effect from zeolite on the nitrification process (Piirtola ***et al.***, 1998, Wahlberg, 1995, Fischer ***et al***, 1978, Hopping, 1978). The main conclusions are that zeolite did not inhibit nitrification in any cases when mixed with sewage. In fact, Fischer ***et al.*** (1978) reported an improvement of the nitrification process achieved by longer sludge retention and lower sludge loading. Another indirect effect that in some cases can improve nitrification is the production in alkalinity that occurs if zeolite undergoes hydrolysis to form kaolinite ($Al_4Si_4O_{10}(OH)_8$).

An interesting observation by Wahlberg (1995) stated that phosphate-containing detergents produced smaller amounts of surfactants, lower toxicity, lower concentration of suspended solids and lower oxygen concentration at the wastewater treatment plants. In fact, that oxygen consumption expressed as BOD_7 was in average three times higher and the suspended solids concentration ten times higher for zeolite containing washing waters than for phosphate-containing washing waters, which would have a great impact for the aeration processes at the wastewater treatment plants.

3.4.3 Reduced hydraulic capacity of secondary clarification tanks

For wastewater treatment plants that will experience an increase of the MLSS concentration in the aeration tanks, the sludge loading of the secondary clarification tanks will increase. Depending on the existing hydraulic capacity, this could result in a decrease of the hydraulic capacity of the plant, since the clarifiers capacity is determined by the amount of sludge that passes them. This phenomenon will probably only affect the wastewater treatment plants that do not perform significant simultaneous precipitation (i.e. they do not have any chemical sludge in the biological sludge) and as a consequence will experience a reduced VSS/SS (Volatile Suspended Solids/Suspended Solids) ratio .

3.4.4 Sludge settling characteristics

Zeolite is a particulate non-degradable substance with a higher density compared with activated sludge flocs. Hence, zeolite will have a positive weighting action on the biological sludge, which will increase the sedimentation velocity of sludge in the settling tank (Piirtola ***et al.***, 1998). Better settling characteristics of sludge will result in improved hydraulic capacity of clarification tanks and less floating sludge discharge in the outlet.

3.4.5 Reduced filtration of sludge

The improved weighting action can be hindered by floc breakdown caused by the ion-exchange capacity of zeolite. This can result in creation of an amorphous form of zeolite in the sludge matrix, which can be harmful for sludge filtration (Cook ***et al.***, 1982). In Piirtola ***et al.*** (1998) this phenomenon was investigated in a pilot scale activated sludge process and it was shown that long contact times (on more than 2 hours) deteriorated filterability of the sludge with more than 40% - probably caused by the complexing metal ions of zeolite – or more likely – by its amorphousness structure of sludge that zeolite creates. Reduced filterability of sludge can result in significant higher sludge volumes after the sludge dewatering process, probably depending on the sludge dewatering technology (centrifuges, belt presses etc.). However, it must be expected that the use of existing or new polymer chemicals partly can account for this problem and reduce the negative effect of reduced filterability of the sludge.

3.5 Conclusions

By introducing a phosphate ban of laundry and automatic dishwashing detergents (powder and tabs) in private households, the phosphate concentration level in municipal wastewater will be significantly reduced. Presently 60-70% of laundry detergents and 100% of automatic dishwashing detergents still contains phosphate and it is estimated that the reduction in phosphate load to wastewater treatment plants could be as high as 46% - a reduction of 2,450 tonnes of phosphorus per year that constitutes 5,350 tonnes phosphorus per year.

Presently, the average phosphorus concentration level in wastewater is 8.9 mg P/l (2004) and this level is expected to be reduced to 4.8 mg P/L as a consequence of a full phosphate substitution in household detergents. The impacts of this on the wastewater treatment plant operation is comprehensive since it probably will result in an almost complete diminishment of chemical precipitation processes, which today accounts for 30-40% of the total phosphorus removal and is responsible for a significant amount of the sludge production at Danish wastewater treatment plants. Furthermore, a significant saving of precipitation chemicals results in a reduction the operation costs in the order of 50 mill. DKK per year. The lower phosphorus concentration is not expected to affect the biological processes – only in cases where the absolute removal of COD is high (more than 800 mg COD/L removed biologically) and the phosphorus concentration is low (4-5 mg P/L) phosphorus shortage could be observed and as a result of this deterioration of the biological performance at the plant.

The sludge composition at wastewater treatment plants will with simultaneous phosphorus precipitation – at first – change by an increase in the VSS/SS ratio, which favours the biological and hydraulic performance of the plants since the presence of chemical sludge virtually can be avoided. However, one of the replacement substances in phosphate-free detergents – zeolite – is expected to affect the sludge composition and sludge behaviour significantly, because zeolite (an inorganic undegradable particulate compound) will accumulate in the sludge matrix with up to 25-30%, depending on the loading to the wastewater treatment plant. This will reduce the organic fraction of the sludge and counteract on the reduced chemical precipitation in the biological process.

The characteristics of sludge settling and dewatering will be affected by the significant increased content of zeolite in the sludge. While the settling characteristics will probably be improved at some plants due to the increased density of zeolite, sludge dewatering will deteriorate vastly unless sludge dewatering chemicals suitable for zeolite containing sludge will be developed/used. Investigations have shown that sludge dewatering can be reduced by at least 40%, which will increase the sludge volumes with the same amount unless methods to dewater sludge as efficiently as today are being developed.

In general, modifications of processes as well as alterations of buildings and other constructions at the wastewater treatment plant may be necessary and consequently expenses may be expected in this regards.

There is no indication that phosphate-free detergents (zeolites) in any way will inhibit the biological processes – in particular the nitrification process.

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Approximations

The amount of households in Denmark is approximately 2,532,000 (Statistics Denmark, 2007) and it is relevant to distinguish between households with one person and households of more than one person.

		Number of laundries per household per year	Number of automatic dish washes per household per year
Number of households in DK	2,532,000		
Number of households with one person	1,094,000	150	0
Number of households with more than one person	1,438,000	400	300

It is assumed that each household of one person has 150 laundries per year and on automatic dish washes, whereas households of more than one person have 400 laundries and 300 automatic dish washes per year.

Recipes for prototypes of laundry detergents and tabs for automatic dishwashing has been set up based on information from SPT and the industry (2007). The prototypes are set up both for the builder system in phosphate-free system and phosphate-containing systems. The concentrations are average values based on more than one input.

Phosphate-free laundry detergent (builder system):

Dose 70 g/laundry

	Weight percent	g per laundry
Zeolite	25	17.5
Sodium silicate	8	5.6
Sodium carbonate	20	14
Citric acid	2.5	1.8
Sodium citrate	7	4.9
Polycarboxylates	1.0	0.7
Phosphonates	0.5	0.4

Phosphate-containing laundry detergent (builder system):

Dose 70 g/laundry

	Weight percent	g per laundry
Phosphates	20	14
Sodium silicate	3	2.1
Sodium carbonate	8	5.6
Sodium citrate	7	4.9
Polycarboxylates	4	2.8

Phosphate-free automatic dishwashing tabs:

Dose 22 g/tabs

	Weight percent	g per wash
Sodium citrate	15	3.3
Citric acid	15	3.3
Sodium silicate	15	3.3
Sodium bicarbonate	23	5.1

Phosphate-containing automatic dishwashing tabs:

Dose 22 g/tabs

	Weight percent	g per wash
Phosphates	45	9.9
Sodium carbonate	15	3.3
Sodium bicarbonate	15	3.3

Appendix B

Ecotoxicological data

Table B.1
Ecotoxicological data for candidate substances for the substitution for phosphate (Highlighted values are used for deriving a PNEC-value)

Substance	Organism	EC_{50}/LC_{50} (mg/L)	NOEC (mg/L)	Time	Reference/(method)
Zeolite 1318-02-1	*Fathead minnow (pimephales promelas)*	>680	>87	96 h	Danish EPA 615
	Fathead minnow		175	30 days	Danish EPA 615
	Daphnia magna	>70 >211-1,000		48 h 21 days	Danish EPA 615
	Daphnia magna		129-1,000	21 days	Danish EPA 615
	Selenastrum carpricornutum	100-1,000		8 h	Danish EPA 615
	Chlorella vulgaris		**70**	8 h	Danish EPA 615
Polycarboxylate 9003-04-7 /9003-01-4 / 52255-49-9	*Crustaceans and fish*	>100-1,000			Danish EPA 615
	Chlorella kessleri	EC_{10} 30-1,000		4-14 days	Danish EPA 615
Sodium citrate (Disodium citrate/ Trisodium citrate) 144-33-2/ 68-04-2	*Poecilia reticulata*	>18,000-32,000		96 h	IUCLID (Method: other)
	Chinook salmon		LOEC 10	96 h	Danish EPA 615
	Daphnia magna	825	80	48 h/ 21 days	Danish EPA 615
	Scenedesmus quadricauda		640	7 days	Danish EPA 615
	Daphnia magna	5,600-10,000		48 h	IUCLID (Method: other)
	Daphnia magna	3,300		24 h	US-EPA

Substance	Organism	EC_{50}/LC_{50} (mg/L)	NOEC (mg/L)	Time	Reference/(method)
	Chlorella vulgaris	>18,000-32,000		96 h	IUCLID (OECD Guideline 201)
Citric acid	*Lepomis macrochirus*	1516		96 h	IUCLID (Method: other)
77-92-9	*Leuciscus idus melanotus*	440		48 h	US-EPA
	Daphnia magna	120		72 h	IUCLID (Method: other)
	Daphnia magna	1,535		24 h	US-EPA
	Scenedesmus quadricauda	640		7 days	IUCLID (Method: other)
Sodium carbonate	*Lepomis macrochirus*	300		96 h	IUCLID (Method: other)
497-19-8	*Lepomis Macrochirus*	300		96 h	US-EPA
	Daphnia magna	265		48 h	IUCLID (Method: other)
	Daphnia magna	**228**		96 h	IUCLID (Method: other)
	Daphnia magna	265		48 h	US-EPA
	Dugesia sp. (flatworm)	341		96 h	US-EPA
	Lymnaea sp. (pond snail)	403		24 h	US-EPA
Sodium bicarbonate	*Lepomis macrochirus*	8,600		96 h	IUCLID (Method: other)
144-55-8	*Daphnia magna*	2,350		48 h	IUCLID (Method: other)
	Nitscheria linearis	**650**		5 d	IUCLID (Method: other)
Sodium silicate	*Branchydanio rerio*	3,185		96 h	IUCLID (OECD Guideline 203)
6834-92-0	*Daphnia magna*	**216**		96 h	IUCLID (Method: other)
Phosphonate	*Ictalurus punctatus*	1,212	924	96 h	IUCLID (OECD Guideline 203)
6419-19-8	*Daphnia magna*	297	125	48 h	IUCLID (OECD Guideline 202)
	Selenastrum capricornitum	19.6	7.4	14 days	IUCLID (OECD Guideline 201)
15827-60-8	*Oncorhynchus mykiss*	180-252	180	96 h	IUCLID (OECD Guideline 203)
	Daphnia magna	242	125	48 h	IUCLID (OECD Guideline 202)
	Selenastrum capricornitum	8.7	5.0	14 days	IUCLID (OECD Guideline 201)
2809-21-4	*Oncorhynchus mykiss*	368	151	96 h	IUCLID (OECD Guideline 203)
	Daphnia magna	527	400	48 h	IUCLID (OECD Guideline 202)
	Chlorella sp.		100	48 h	IUCLID (Method:other)

Substance	Organism	EC_{50}/LC_{50} (mg/L)	NOEC (mg/L)	Time	Reference/(method)
	Selenastrum sp.		3.0	21 days	IUCLID (Bottle test, US-EPA)
Sodium tartrate 868-18-8	*Fish*	1,000			Danish EPA QSAR
	Daphnia	893			Danish EPA QSAR
	Algae	864			Danish EPA QSAR
Sodium gluconate 527-07-1	*Fish*	100			Danish EPA QSAR
	Daphnia	148			Danish EPA QSAR
	Algae	1,260			Danish EPA QSAR
MGDA (Methyl glycin diacetic acid)	-	-	-	-	-
IDS (Iminodisuccinate) 144538-83-0	*Fish*	LC_0: ≥ 82.6		96 h	Baypure (2009)
	Fish	LC_0: ≥ 12.0		14 days	Baypure (2009)
	Daphnia	EC_0: ≥ 84.0		48 h	Baypure (2009)
	Daphnia	EC_0: ≥ 11.7		21 days	Baypure (2009)
	Algae		22.8	72 h	Baypure (2009)
GLDA (GLutamic acid Diacetic Acid)	-	-	-	-	-

Danish EPA 615: Environmental Project No. 615, 2001 [in Danish].
Danish EPA QSAR: QSAR calculations from Danish EPA
Baypure (2009). www.baypure.com August 2009. Data on Baypure^{TM} CX 100 solid
- No data available

ECO Lab model

Modelling the complexity of sewage treatment systems in Europe is not possible in EUSES, which cannot include combinations of highly sophisticated and less sophisticated STPs (Sewage Treatment Plants). Therefore, an emission/inventory model was developed with the aim to estimate the emission fractions of single detergent ingredients from household use on a country level. The model core is based on the national wastewater distribution pattern statistics. These data combined with the overall removal fractions by various types of sewage treatment systems enable the estimation of the emission fraction from complex sewage treatment systems consisting of many types of sewage treatment. The following types of treatments are considered in the inventory model:

E1: Mini STPs
E2: Septic tanks
E3: STPs with primary treatment
E4: STPs with secondary treatment
E5: STPs with tertiary treatment
E6: Direct emissions

Once a substance is emitted to surface water, a number of fate and transport processes will take place, e.g. advection, dispersion, sedimentation, degradation.

The modelling was carried out by combining a hydraulic model for the description of the water movements and a fate model. The fate model was programmed in an ECO Lab template and combined with the hydraulic model MIKE 21.

The hydraulic model needs a specification of the water body and meteorological data.

The Little Belt was chosen for the Danish surface water scenario, and meteorological data for April 2004 was used. Furthermore, the model needs a specification of the emission sources with respect to location and size. The specification of the emission sources with respect to position is illustrated in Figure C.1. Only STPs with tertiary and primary treatment are included in the scenario and only one source with direct discharge (summer cottage area) was included in the scenario.

Figure C.1
Position of emission sources

The fate model includes the following fate processes:

Volatilization, where the model suggested by Schwarzenbach et al. (1993) is used. This model accounts for the effects of diffusion rates in water and air, Henry's law constant and air velocity on the rate of volatilization.

Net sedimentation, where a linear rate of sedimentation of suspended matter is assumed. Only substances bound to the suspended matter are assumed to sedimentate.

Biodegradation, where first order rate degradation kinetics are assumed. The influence of temperature on the biodegradation rate constant is described through an Arrhenius-like description: $k_{bio}(t) = k_{bio}(t_0)\cdot e^{A(t-t_0)}$, where $k_{bio}(t)$ is the rate constant at temperature t, t_0 is the reference temperature at which the reference biodegradation rate constant $k_{bio}(t_0)$ is specified, and A is a temperature coefficient.

Photolysis, where the rate of photolysis is described by a first order degradation rate constant at the water surface and by the absorption of light through the water column.

Diffusion of the chemicals from the water column to the sediment is neglected. However, this process may be important for environments not previously exposed with a particular substance; if surfaces for sorption in the sediment are unsaturated (this situation is not likely for high volume chemicals). The concentration of the substances in top layer of the sediment is calculated by assuming that the sediment surface layer is in equilibrium with the overlying water.

The output of the model is predicted concentrations in surface water varying in time and space. For the further risk assessment, the following approach was used:

For each emission source, the average and maximum concentration in a volume around the point of discharge was derived

The 90th percentile concentration was derived for each type of emission source

The overall PEC to be used in the risk assessment was found by a weighted average (with respect to percentage of population connected to the type of wastewater treatment).

EUSES

Input data and output data for the estimations of PEC in the EU TGD 2003 Risk Assessment Spreadsheet Model (2007) for the following substances:

Zeolit
Sodium silicate
Phosphonate
IDS (Iminodisuccinate)

INPUT

REGION IDENTIFICATION

General name	Default EUSES	▼	-

SUBSTANCE IDENTIFICATION

General name		Zeolit	
CAS no.		1318-02-1	

PHYSICAL-CHEMICAL SUBSTANCE PROPERTIES

Molecular weight		200	$g.mol^{-1}$
Melting point		1200	°C
Vapour pressure at the temperature of the data set		1,0E-10	Pa
Temperature at which vapour pressure was measured		20	°C
Water solubility at the temperature of the data set		1,0E-10	$mg.L^{-1}$
Temperature at which solubility was measured		20	°C
Octanol-water partition coefficient		1,0E-04	-
Chemical class for Koc-QSAR	Non hydrophobics	▼	-
Organic carbon - water partition coefficient			L.kg-1

DEGRADATION AND TRANSFORMATION RATES

Characterization

Biodegradability test result	not biodegradable		▼
Rate constant for degradation in STP			d-1
Total rate constant for degradation in surface water at env. temp			d^{-1}
Total rate constant for degradation in marine water at env. temp			d-1
Total rate constant for degradation in bulk sediment at env. temp			d-1
Rate constant for degradation in air			d-1
Total rate constant for degradation in bulk soil at env. temp			d-1

EMISSIONS

Tonnages

Tonnage in EU		1,2E+01	$tonnes.yr^{-1}$

Fraction of EU production volume in Region	1,000	-
Release fractions		
Fraction of tonnage released to air	0,00	-
Fraction of tonnage released to waste water	1,00	-
Fraction of tonnage released to surface water	0,00	-
Fraction of tonnage released to industrial soil	0,00	-
Fraction of tonnage released to agricultural soil	0,00	-
Emission days		
Fraction of the main local source	0,0	-
Number of emission days per year	365	$d.yr^{-1}$
Local release rates		
Local emission to air during episode	0,0E+00	$kg.d^{-1}$
Local emission to wastewater during episode	3,2E+01	$kg.d^{-1}$

OUTPUT

PREDICTED CONCENTRATIONS

PECs **Zeolit**

Regional PEC in surface water (total)	2,4E-05	$mg_c.L^{-1}$
Regional PEC in sea water (total)	2,2E-06	$mg_c.L^{-1}$
Regional PEC in air (total)	5,2E-07	$mg_c.m^{-3}$
Regional PEC in agricultural soil (total)	2,9E-09	$mg_c.kg_{wwt}^{-1}$
Regional PEC in natural soil (total)	2,1E-09	$mg_c.kg_{wwt}^{-1}$
Regional PEC in industrial soil (total)	2,1E-09	$mg_c.kg_{wwt}^{-1}$
Regional PEC in sediment (total)	1,4E-05	$mg_c.kg_{wwt}^{-1}$
Regional PEC in sea water sediment (total)	1,3E-03	$mg_c.kg_{wwt}^{-1}$
Annual average local PEC in air (total)	6,1E-03	$mg_c.m^{-3}$
Local PEC in surface water during emission episode (dissolved)	5,0E-01	$mg_c.L^{-1}$
Annual average local PEC in surface water (dissolved)	5,0E-01	$mg_c.L^{-1}$
Local PEC in fresh water sediment during emission episode	3,9E-01	$mg_c.kg_{wwt}^{-1}$
Local PEC in sea water during emission episode (dissolved)	5,0E-02	$mg_c.L^{-1}$
Annual average local PEC in sea water (dissolved)	5,0E-02	$mg_c.L^{-1}$
Local PEC in marine sediment during emission episode	1,8E+01	$mg_c.kg_{wwt}^{-1}$
Local PEC in agricultural soil, averaged over 30 days	3,3E-07	$mg_c.kg_{wwt}^{-1}$
Local PEC agricultural soil, averaged over 180 days	2,0E-07	$mg_c.kg_{wwt}^{-1}$
Local PEC in grass land, averaged over 180 days	1,8E-07	$mg.kg_{wwt}^{-1}$

INPUT

REGION IDENTIFICATION

General name	Default EUSES	▼	-

SUBSTANCE IDENTIFICATION

General name	Sodium silicate	
CAS no.	6834-92-0	

PHYSICAL-CHEMICAL SUBSTANCE PROPERTIES

Molecular weight		124	g.mol^{-1}
Melting point		1000	$^{\circ}$C
Vapour pressure at the temperature of the data set		1,0E-10	Pa
Temperature at which vapour pressure was measured		20	$^{\circ}$C
Water solubility at the temperature of the data set		2,0E+05	mg.L^{-1}
Temperature at which solubility was measured		20	$^{\circ}$C
Octanol-water partition coefficient		1,0E-04	-
Chemical class for Koc-QSAR	Non hydrophobics	▼	-
Organic carbon - water partition coefficient			L.kg-1

DEGRADATION AND TRANSFORMATION RATES

Characterization

Biodegradability test result	not biodegradable	▼	
Rate constant for degradation in STP			d-1
Total rate constant for degradation in surface water at env. temp			d^{-1}
Total rate constant for degradation in marine water at env. temp			d-1
Total rate constant for degradation in bulk sediment at env. temp			d-1
Rate constant for degradation in air			d-1
Total rate constant for degradation in bulk soil at env. temp			d-1

EMISSIONS

Tonnages

Tonnage in EU	3,7E+00	tonnes.yr^{-1}

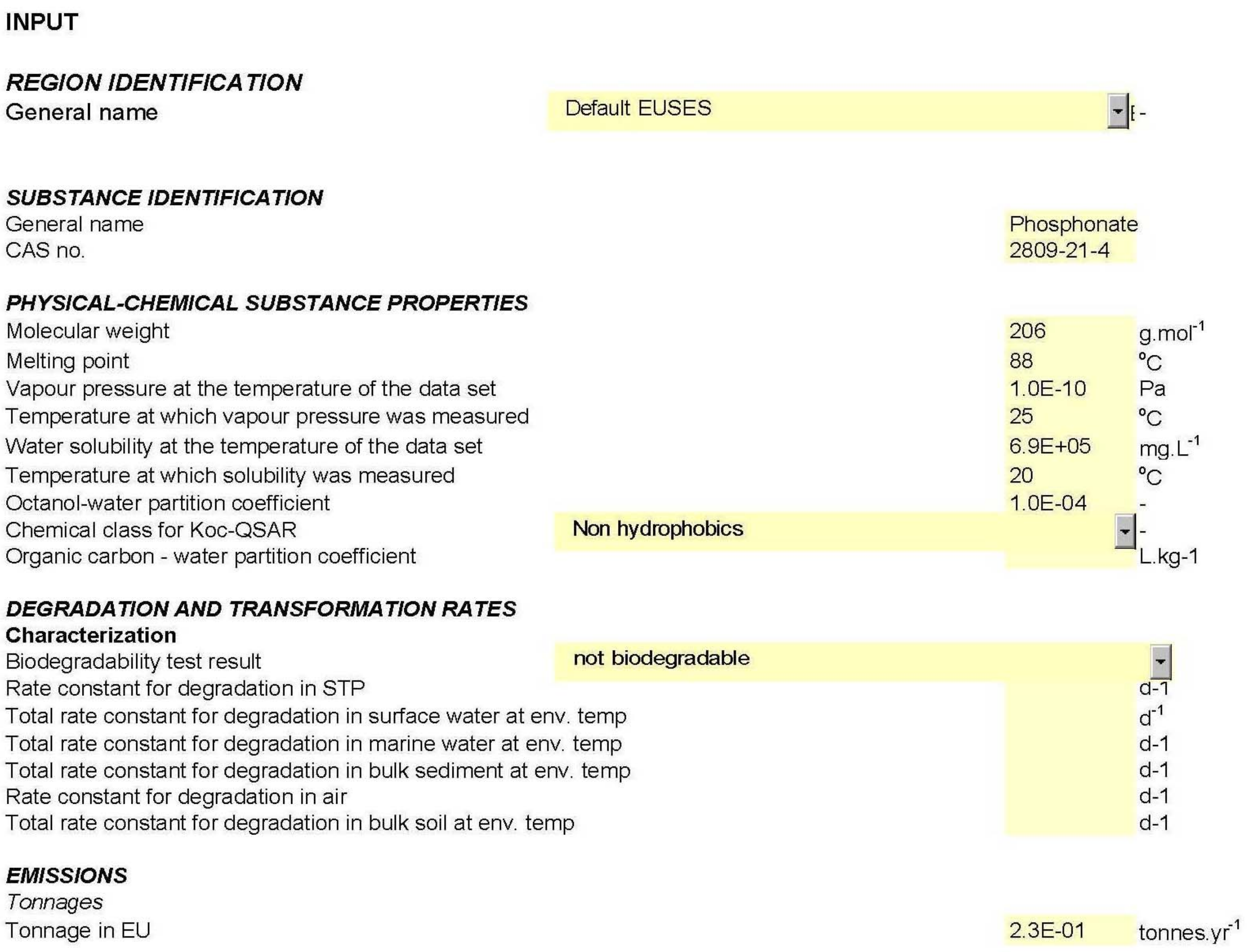
Fraction of EU production volume in Region	1,000	-
Release fractions		
Fraction of tonnage released to air	0,00	-
Fraction of tonnage released to waste water	1,00	-
Fraction of tonnage released to surface water	0,00	-
Fraction of tonnage released to industrial soil	0,00	-
Fraction of tonnage released to agricultural soil	0,00	-
Emission days		
Fraction of the main local source	0,0	-
Number of emission days per year	365	$d.yr^{-1}$
Local release rates		
Local emission to air during episode	0,0E+00	$kg.d^{-1}$
Local emission to wastewater during episode	1,0E+01	$kg.d^{-1}$

OUTPUT

PREDICTED CONCENTRATIONS

PECs **Sodium Silicate**

Regional PEC in surface water (total)	7,6E-05	$mg_{c}.L^{-1}$
Regional PEC in sea water (total)	7,7E-06	$mg_{c}.L^{-1}$
Regional PEC in air (total)	1,4E-31	$mg_{c}.m^{-3}$
Regional PEC in agricultural soil (total)	4,6E-10	$mg_{c}.kg_{wwt}^{-1}$
Regional PEC in natural soil (total)	2,0E-18	$mg_{c}.kg_{wwt}^{-1}$
Regional PEC in industrial soil (total)	2,0E-18	$mg_{c}.kg_{wwt}^{-1}$
Regional PEC in sediment (total)	4,6E-05	$mg_{c}.kg_{wwt}^{-1}$
Regional PEC in sea water sediment (total)	4,7E-03	$mg_{c}.kg_{wwt}^{-1}$
Annual average local PEC in air (total)	2,1E-18	$mg_{c}.m^{-3}$
Local PEC in surface water during emission episode (dissolved)	5,1E-01	$mg_{c}.L^{-1}$
Annual average local PEC in surface water (dissolved)	5,1E-01	$mg_{c}.L^{-1}$
Local PEC in fresh water sediment during emission episode	4,0E-01	$mg_{c}.kg_{wwt}^{-1}$
Local PEC in sea water during emission episode (dissolved)	5,1E-02	$mg_{c}.L^{-1}$
Annual average local PEC in sea water (dissolved)	5,1E-02	$mg_{c}.L^{-1}$
Local PEC in marine sediment during emission episode	1,8E+01	$mg_{c}.kg_{wwt}^{-1}$
Local PEC in agricultural soil, averaged over 30 days	1,8E-04	$mg_{c}.kg_{wwt}^{-1}$
Local PEC agricultural soil, averaged over 180 days	8,7E-05	$mg_{c}.kg_{wwt}^{-1}$
Local PEC in grass land, averaged over 180 days	1,9E-05	$mg.kg_{wwt}^{-1}$



INPUT

REGION IDENTIFICATION

General name	Default EUSES	-

SUBSTANCE IDENTIFICATION

General name	Phosphonate	
CAS no.	2809-21-4	

PHYSICAL-CHEMICAL SUBSTANCE PROPERTIES

Molecular weight	206	$g.mol^{-1}$
Melting point	88	°C
Vapour pressure at the temperature of the data set	1.0E-10	Pa
Temperature at which vapour pressure was measured	25	°C
Water solubility at the temperature of the data set	6.9E+05	$mg.L^{-1}$
Temperature at which solubility was measured	20	°C
Octanol-water partition coefficient	1.0E-04	-
Chemical class for Koc-QSAR	Non hydrophobics	-
Organic carbon - water partition coefficient		L.kg-1

DEGRADATION AND TRANSFORMATION RATES

Characterization

Biodegradability test result	not biodegradable	
Rate constant for degradation in STP		d-1
Total rate constant for degradation in surface water at env. temp		d^{-1}
Total rate constant for degradation in marine water at env. temp		d-1
Total rate constant for degradation in bulk sediment at env. temp		d-1
Rate constant for degradation in air		d-1
Total rate constant for degradation in bulk soil at env. temp		d-1

EMISSIONS

Tonnages

Tonnage in EU	2.3E-01	$tonnes.yr^{-1}$

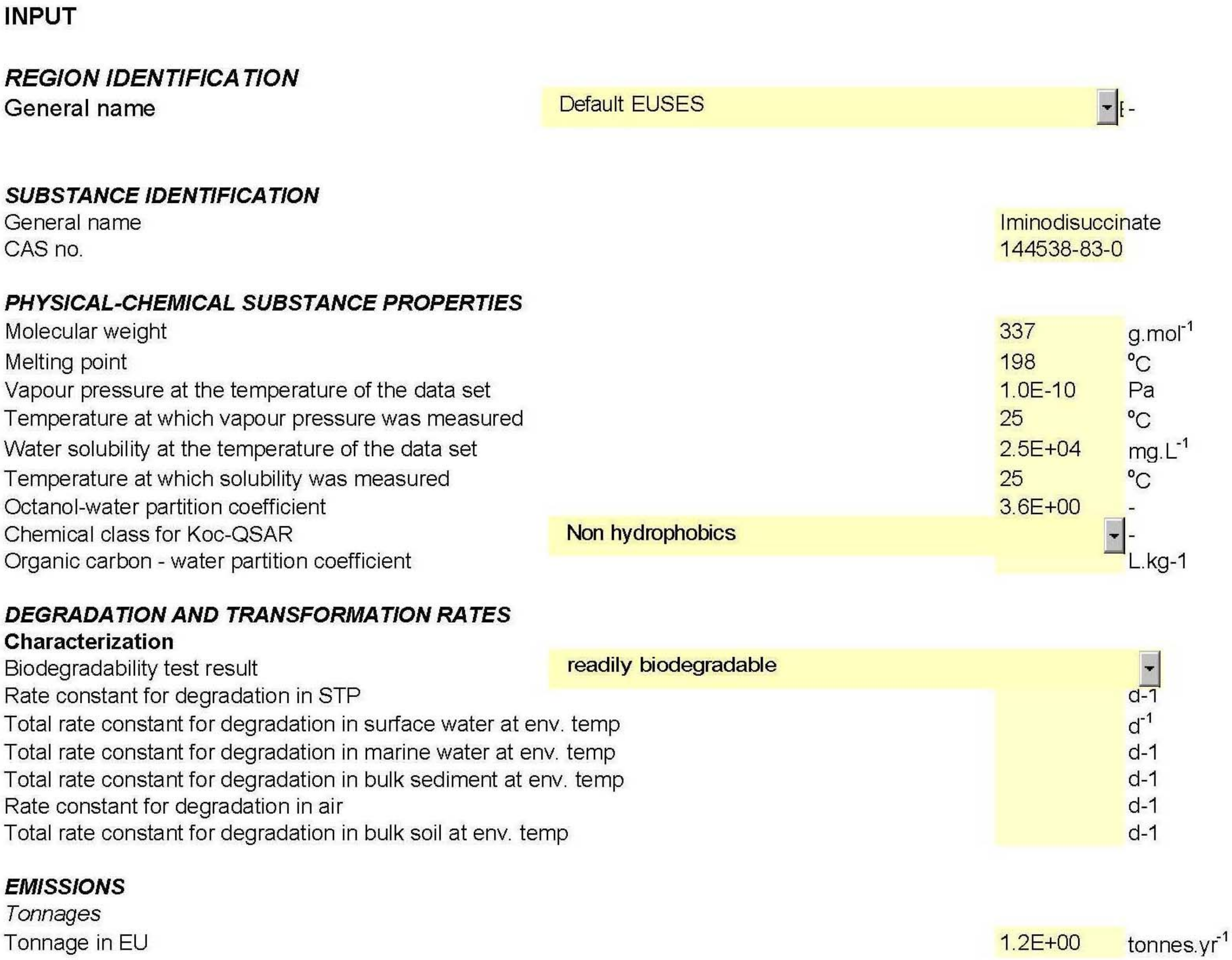
Fraction of EU production volume in Region	1.000	-
Release fractions		
Fraction of tonnage released to air	0.00	-
Fraction of tonnage released to waste water	1.00	-
Fraction of tonnage released to surface water	0.00	-
Fraction of tonnage released to industrial soil	0.00	-
Fraction of tonnage released to agricultural soil	0.00	-
Emission days		
Fraction of the main local source	0.0	-
Number of emission days per year	365	d.yr^{-1}
Local release rates		
Local emission to air during episode		kg.d^{-1}
Local emission to wastewater during episode	6.4E-01	kg.d^{-1}

OUTPUT

PREDICTED CONCENTRATIONS

PECs **Phosphonate**

Regional PEC in surface water (total)	4.7E-06	$mg_c.L^{-1}$
Regional PEC in sea water (total)	4.8E-07	$mg_c.L^{-1}$
Regional PEC in air (total)	5.0E-28	$mg_c.m^{-3}$
Regional PEC in agricultural soil (total)	2.9E-11	$mg_c.kg_{wwt}^{-1}$
Regional PEC in natural soil (total)	3.5E-20	$mg_c.kg_{wwt}^{-1}$
Regional PEC in industrial soil (total)	3.5E-20	$mg_c.kg_{wwt}^{-1}$
Regional PEC in sediment (total)	2.9E-06	$mg_c.kg_{wwt}^{-1}$
Regional PEC in sea water sediment (total)	2.9E-04	$mg_c.kg_{wwt}^{-1}$
Annual average local PEC in air (total)	4.6E-20	$mg_c.m^{-3}$
Local PEC in surface water during emission episode (dissolved)	3.2E-02	$mg_c.L^{-1}$
Annual average local PEC in surface water (dissolved)	3.2E-02	$mg_c.L^{-1}$
Local PEC in fresh water sediment during emission episode	2.5E-02	$mg_c.kg_{wwt}^{-1}$
Local PEC in sea water during emission episode (dissolved)	3.2E-03	$mg_c.L^{-1}$
Annual average local PEC in sea water (dissolved)	3.2E-03	$mg_c.L^{-1}$
Local PEC in marine sediment during emission episode	1.2E+00	$mg_c.kg_{wwt}^{-1}$
Local PEC in agricultural soil, averaged over 30 days	1.1E-05	$mg_c.kg_{wwt}^{-1}$
Local PEC agricultural soil, averaged over 180 days	5.4E-06	$mg_c.kg_{wwt}^{-1}$
Local PEC in grass land, averaged over 180 days	1.2E-06	$mg.kg_{wwt}^{-1}$



INPUT

REGION IDENTIFICATION		
General name	Default EUSES	-
SUBSTANCE IDENTIFICATION		
General name	Iminodisuccinate	
CAS no.	144538-83-0	
PHYSICAL-CHEMICAL SUBSTANCE PROPERTIES		
Molecular weight	337	g.mol^{-1}
Melting point	198	°C
Vapour pressure at the temperature of the data set	1.0E-10	Pa
Temperature at which vapour pressure was measured	25	°C
Water solubility at the temperature of the data set	2.5E+04	mg.L^{-1}
Temperature at which solubility was measured	25	°C
Octanol-water partition coefficient	3.6E+00	-
Chemical class for Koc-QSAR	Non hydrophobics	-
Organic carbon - water partition coefficient		L.kg-1
DEGRADATION AND TRANSFORMATION RATES		
Characterization		
Biodegradability test result	readily biodegradable	
Rate constant for degradation in STP		d-1
Total rate constant for degradation in surface water at env. temp		d^{-1}
Total rate constant for degradation in marine water at env. temp		d-1
Total rate constant for degradation in bulk sediment at env. temp		d-1
Rate constant for degradation in air		d-1
Total rate constant for degradation in bulk soil at env. temp		d-1
EMISSIONS		
Tonnages		
Tonnage in EU	1.2E+00	tonnes.yr^{-1}

Fraction of EU production volume in Region	1.000	-
Release fractions		
Fraction of tonnage released to air	0.00	-
Fraction of tonnage released to waste water	1.00	-
Fraction of tonnage released to surface water	0.00	-
Fraction of tonnage released to industrial soil	0.00	-
Fraction of tonnage released to agricultural soil	0.00	-
Emission days		
Fraction of the main local source	0.0	-
Number of emission days per year	365	$d.yr^{-1}$
Local release rates		
Local emission to air during episode		$kg.d^{-1}$
Local emission to wastewater during episode	3.2E+00	$kg.d^{-1}$

OUTPUT

PREDICTED CONCENTRATIONS

PECs **Iminodisuccinate**

Regional PEC in surface water (total)	3.2E-06	$mg_c.L^{-1}$
Regional PEC in sea water (total)	3.1E-07	$mg_c.L^{-1}$
Regional PEC in air (total)	5.9E-26	$mg_c.m^{-3}$
Regional PEC in agricultural soil (total)	2.1E-08	$mg_c.kg_{wwt}^{-1}$
Regional PEC in natural soil (total)	2.1E-18	$mg_c.kg_{wwt}^{-1}$
Regional PEC in industrial soil (total)	2.1E-18	$mg_c.kg_{wwt}^{-1}$
Regional PEC in sediment (total)	3.1E-06	$mg_c.kg_{wwt}^{-1}$
Regional PEC in sea water sediment (total)	3.0E-04	$mg_c.kg_{wwt}^{-1}$
Annual average local PEC in air (total)	2.4E-18	$mg_c.m^{-3}$
Local PEC in surface water during emission episode (dissolved)	2.0E-02	$mg_c.L^{-1}$
Annual average local PEC in surface water (dissolved)	2.0E-02	$mg_c.L^{-1}$
Local PEC in fresh water sediment during emission episode	2.5E-02	$mg_c.kg_{wwt}^{-1}$
Local PEC in sea water during emission episode (dissolved)	2.0E-03	$mg_c.L^{-1}$
Annual average local PEC in sea water (dissolved)	2.0E-03	$mg_c.L^{-1}$
Local PEC in marine sediment during emission episode	1.1E+00	$mg_c.kg_{wwt}^{-1}$
Local PEC in agricultural soil, averaged over 30 days	7.9E-03	$mg_c.kg_{wwt}^{-1}$
Local PEC agricultural soil, averaged over 180 days	2.4E-03	$mg_c.kg_{wwt}^{-1}$
Local PEC in grass land, averaged over 180 days	8.7E-04	$mg.kg_{wwt}^{-1}$