Tributyltin - TBT

SEDIMENT EQS DERIVATION

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Stockholm University

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Preface

The Department of Environmental Science and Analytical Chemistry (ACES) at Stockholm University was commissioned, by the Swedish Agency for Marine and Water Management (SwAM), to prepare a Water Framework Directive (WFD) sediment Environmental Quality Standard (EQS) dossier in English for Tributyltin (TBT). Compared to the existing European EQS dossier for tributyltin compounds where sediment toxicity is also addressed this dossier includes new data delivered to SwAM by Golder (in 2013 and 2014) and calculations performed by SwAM. Besides translating the information from Golder and the calculations performed by SwAM from Swedish into English, correction of typos and restructuring of text has been done to fit into the EQS dossier format used at the European level.

The report was prepared by Sara Sahlin and Marlene Ågerstrand.

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1. INTRODUCTION

Tributyltin (TBT) compounds are included in the list of priority substances for which Environmental Quality Standards (EQS) are implemented for surface water through the Directive 2008/105/EC (the EQS Directive). The EQS dossier for TBT included a preliminary $QS_{sediment}$ derived using the Equilibrium partitioning (EqP) approach, with QS set to 0.02 µg/kg (European Commission 2005). This value, however, was considered preliminary and was not implemented in the Directive 2008/105/EC. Nevertheless, TBT tends to strongly bind to sediment, and it is therefore not degraded to the same extent as in water. Because TBT accumulates in sediment, benthic organisms can be assumed to be exposed to higher levels compared to pelagic organisms.

The Swedish Agency of Marine and Water Management (SwAM) has established a national EQS for TBT in sediment from a $QS_{sediment}$ that is based on ecotoxicity studies on benthic organisms (HVMFS 2013:19). The background data on Koc and toxicity studies associated with the establishment of the $QS_{sediment}$ was collected and evaluated by the consultant Golde*r* in 2013 and 2014. SwAM calculated the EQS for TBT in sediment in collaboration with experts at the Swedish Environmental Protection Agency. The references and calculations were included in an annex that was sent on public consultation[1] in Sweden in July 2014. After the consultation, the sediment EQS was included in national legislation in 2015 (by HVMFS 2015:4 revising HVMFS 2013:19)[2].

TBT: Chemical identity	
CAS no.	36643-28-4 (cation)
Kow	3.1-4.1[1] (Log Kow)
Koc	4.6-5.3 (log Koc)[2] (≈ 40000 – 200 000 Koc) 300-1500000[1]

1 = European Commission, 2005. 2 = Brändil et al., 2009.

[1] Available from SwAM referring to file no 3383-17.

[2] Havs- och vattenmyndighetens föreskrifter (HVMFS 2013:19) om klassificering och miljökvalitetsnormer avseende ytvatten.

2. PROPOSED QUALITY STANDARDS (QS)

2.1 Environmental Quality Standard (EQS)

The proposed sediment EQS for TBT is 1.6 µg/kg dry weight (expressed as 5% organic carbon) considering both marine and freshwater sediments. The TOC content of 5% represents a standard sediment according to European Communities (2011). This value is consistent with Swedish coastal levels of TOC (e.g. Jonsson et al., 2003), although deviations may occur (from a few percent to approximately 20%). In cases where TOC differs from 5%, the measured TBT concentration is multiplied with the ratio of TOC (5/ actual TOC level), before comparing to the EQS.

	Value	Comments
Proposed $EQS_{sediment}$ [$\mu g.kg^{-1}$ at 5% TOC]	**1.6**	**See section 3.2**
$QS_{sediment}$ based on EqP [$\mu g.kg^{-1}$ at 5% TOC]	0.4	See section 3.4

3. EFFECTS AND QUALITY STANDARDS

In the literature search conducted in 2013, 10 studies were available investigating toxicity to 9 freshwater species, 3 marine species and marine meiobenthic communities (table S1). All studies were assessed as *reliable with restrictions* using the Klimisch method (Klimisch et al., 1997). The total dataset revealed that the species showing highest sensitivity to TBT was the freshwater Gastropoda: *Potamopyrgus antipodarum.*

The available marine sediment data suggest that marine species are less sensitive compared to freshwater species. However, the marine dataset lacked data for the most sensitive taxonomic group; Gastropoda. It was therefore assumed that the use of the available marine data in the derivation would lead to an underestimation of QS_{marine}. When marine ecotoxicity data is lacking, a larger AF is required compared to freshwater sediment derivation. Nevertheless, in the substance datasheet from the European Commission (2005) it was concluded that freshwater and marine species show similar sensitivity to TBT compounds. Furthermore, TBT in marine water was assumed to have reduced bioavailability due to the salinity and increased pH. Based on this, data for freshwater and marine species were pooled and the derived EQS is assumed to protect organisms in both marine and freshwater sediments.

3.1 Critical study

Duft et al. (2003) investigated effects from TBT exposure on the freshwater Gastropoda *Potamopyrgus antipodarum* using artificial spiked sediment with a duration of 2, 4 and 8 weeks. The most sensitive endpoint was the number of new embryos (without shells) after 4 weeks of exposure. Seven concentrations were used in the bioassay and the effect was seen already at the lowest concentration (EC_{10} of 0.98 μg/kg dw). The EC_{10} was higher after 8 weeks compared to 4 weeks (2.98 μg/kg dw), which was assumed to be due to that TBT sorb to the sediment after longer duration. It is plausible that the bioavailability in the environment is reduced with time (i.e. "ageing"). In addition, the dose-response curve was clearer after 8 weeks compared to 4 weeks and analysis of sediment concentration was not undertaken until week 8. Based on this, the 8 week EC_{10} was assumed to be more reliable. This EC_{10} was recalculated to 16 μg/kg dw expressed as 5% TOC (a TOC content of 2.3% was used in the bioassay).

3.2 $QS_{sediment}$ derivation

An AF of 10 was assessed as sufficient, since effect data for three chronic freshwater studies were available investigating at least three sediment-dwelling species representing different living-conditions (*Chironomus riparius, Monoporeia affinis, Hyalella azteca, Hexagenia limbata, Physella gyrina, Tubifex tubifex, Daphnia magna)* (European Communities, 2011). The marine dataset was also assumed to fulfill the use of AF 10 since four chronic marine studies were available (*Echinocardium cordatum, Amandia brevis, Corophium volutator,* and benthic nematode communities) (European Communities, 2011).

Using the critical study for *Potamopyrgus antipodarum* with EC_{10} of 16 μg/kg dw and AF 10 resulted in a QS of 1.6 μg/kg dw at 5% TOC. This EQS is assumed to protect both freshwater and marine sediment-dwelling species.

3.3 Field evidence

When deriving EQS for the sediment compartment, field- and mesocosms data should be considered according to the European Communities (2011). Analysis of effects caused by TBT (i.e. imposex of Gastropoda) and TBT levels in sediment were available from the West coast of Sweden (marine sediment).

TBT gives raise to imposex in several water-living gastropods, which means that females becomes masculinized (developing penis). The level of imposex is assessed based on the stage of the vas deferens formation. The formation is assessed based on up to 9 different stages depending on species, where 0 is the normal female without vas deferens. For the Nassariidae (family belonging to Gastropoda) there are 5 different stages (0-4) and a vas deferens sequence index (VDSI) of ≤ 0.3 is considered unaffected (OSPAR, 2010).

Field studies analyzing effects of TBT of the snail Nassariidaeand levels of TBT in sediment has been carried out in marinas, located in Fiskebäckskil and Grebbestad (Magnusson et al., 2012). Lowest levels of TBT (1.8 μg/kg dw) and lowest degree of imposex (VDSI of 0.3) was detected in Fiskebäckskil, with a general decrease of imposex and TBT concentrations with distance from the inner submarine. The lowest VDSI (0.4) in Grebbestad was observed in the reference site where TBT was measured at a level of 2.6 μg/kg dw. Higher VDSI (1.6 and 0.5) was detected at other locations, however, these locations had reduced levels of TBT detected in the sediment (approximately 0.5 μg/kg dw). The TOC content was not analyzed but it is plausible that TOC (i.e. the bioavailability) could explain these unexpected results (i.e. higher levels of TBT did not show increased effect in Grebbestad). Based on these field observations it was concluded that a 5% normalized value of 1.6 μg/kg dw is reasonable since effect levels in field studies were in the same range.

This EQS was further supported by the threshold value given in the integrated assessment of TBT-levels within OSPAR (2008), of which sediment levels under 2 μg/kg is assumed to correspond to VDSI < 0.3 (of Nassariidae).

3.4 $QS_{sediment}$ derivation using Equilibrium partitioning (EqP)

Calculation based on the surface water $EQS_{fw\ eco}$ using the Equilibrium partitioning approach was also undertaken, according to European Communities (2011) (although, it is stipulated that EQS primarily should be based on ecotoxicity studies rather than such calculation). In this context, EqP calculation was problematic due to the large variation of Koc reported in the literature. Due to the ionizable properties of TBT the partitioning between water and sediment is highly influenced by TOC, pH, salinity and also the concentration of TBT (Langston and Pope, 1995). It can therefore be assumed that TBT is more tightly bound to marine sediments compared to freshwater sediments with lower pH.

In the dossier from the European Commission (2005), the reported Koc varied between 300 and 150,000 and the EqP calculation was based on 1084, which resulted in a value of 0.02 μg/kg dw. This value is likely highly conservative, taking into consideration the conditions normally prevailing in the environment. A complementary literature search was performed aiming to compile reliable Koc values representing Swedish conditions (table S2). The Koc of 40 000 (log value= 4.6) was selected for the calculation, based on a Norwegian investigation (Brändli et al., 2009). Based on this Koc the EqP calculations resulted in an EQS of 0.4 μg/kg dw, which is four-fold lower than the EQS value based on ecotoxicity studies (see section 9 for EpP calculations), but 20-fold higher than the preliminary value set by the European Commission (2005).

4. IDENTIFICATION OF ISSUES RELATING TO UNCERTAINTY IN RELATION TO THE QSs DERIVED

Not specified.

5. IDENTIFICATION OF ANY POTENTIAL IMPLEMENTATION ISSUES IN RELATION TO THE QSs DERIVED

A standard quantification limit of TBT in sediment is 1 μg/kg. The EQS of 1.6 μg/kg does therefore not fulfil the requirements of quantification limits of EQS times 0.3, set according to 2009/90/EG (or NFS 2006:11). However, the quantification limit for water is significantly worse in relation to the EQS. Analytical methods can normally analyze 0.001 μg/L, while the EQS is 0.0002 μg/L.

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7. SUPPORTIVE INFORMATION: ECOTOXICITY DATA

Tabell S1. Sediment ecotoxicity studies of TBT. Critical data is marked in bold.

Organism	Method	Limnic / Marine	Organic carbon[1]; sediment type	Duration	Endpoint/s	Effect conc (µg TBT/kg dw)[2]	Physico-chemical conditions	Validity/relevance	Reference
Chironomus riparius Obtained from a mass culture, established in 2009.	TBT was tested in three exposure groups; low medium and high, a control and a solvent with four replicates each (50 test organisms/ replicate). Sediment was spiked with TBT chloride and placed in aerated aquaria, with 1250 g of sed and 3000 mL water. Nominal conc: 30, 90 and 180 µg/kg Measured conc: 24, 117 and 231 µg/kg	Limnic	4 % LOI (approx 2.3 % TOC) Natural sediment (Finnish caolin clay, Kerapo Helsinki) and fine sand (Biltema)	Single (> 15 d) and multi (5) generations test.	- life history traits (development time, survival, fecundity and weight) - immune response	Single generation: Lengthened larval development: LOEC = 24 µg/kg [52 at 5 % TOC] Reduction in larval survival: LOEC = 114 µg/kg [250 at 5 % TOC] Adult bodyweight was reduced by TBT contamination, but no significant effect was obseved under the highest conc, due to lack of data. Adult fecundity increased in medium and high concentrations. Hemocyte densities were reduced by TBT, while no significant effect was observed for PO activity. In the single generation test TBT affected all tested endpoints compared to control. The effect of continous exposure to TBT over five generations varied between the different TBT treatments, supported by a statistically significant interaction	pH: 7.9 - 8.4 18 °C (ambient temperature)	Klimish score: 2 Ecologically relevant study. Generally, relevant for Swedish conditions. However, relatively high pH. Temperature relevant for summer condition. Only three different TBT test concentrations, thus LOEC and NOEC may be under- and overestimated respectively.	Lilley et al 2012

Organism	Method	Limnic / Marine	Organic carbon[1]; sediment type	Duration	Endpoint/s	Effect conc (µg TBT/kg dw)[2]	Physico-chemical conditions	Validity/relevance	Reference
						between generation time and TBT treatment. The results showed that TBT had both first generation and multigeneration effects on all tested parameters. A five generation exposure lead to extintion in all treatments.			
Monoporeia affinis Natural micro and meiofauna. collected at 3 cm depth in late October 2008 at Björkfjärden in lake Mälaren.	Organisms were exposed to TBT (Tributyltin TBTO (Sigma-Aldrich) during gonad maturation, in microcosms with spiked sediments under static conditions. Each microcosm had a bottom layer of 150 mL sediment with natural composition of micro- and meiofauna from the collection site and 1 L freshwater. The water was aerated throughout the test. The experiment lasted for 5 weeks with the following exposure groups each consisting of seven microcosms (replicates) with 26 adults in each: (A) Control, (B) 70 g TBT/kg sediment dw and (C) 170 g TBT/kg sediment dw. In total there were 21 replicates and 546 animals. Nominal concentrations: Control: 0 ng TBT/g dw Low: 100 ng TBT/g dw High: 250 ng TBT/g dw	Limnic	LOI 7.6 ± 0.02 % (approx 4.4 % TOC) Natural sediments. Sediment compositio n at 3 cm depth (in Björkfjärde n in lake Mälaren) was detemined to 0.8 % sand, 31 % silt and 68 % clay.	35 d	Survival Reproduction Dead oocytes in female gonads Parasites (numbers of infected organisms)	Survival NOEC: 170 µg TBT/kg dw Female sexual maturation NOEC: 170 µg TBT/kg dw Male sexual maturation Borderline statistical significant increase in the proportion of sexually mature males Dead oocytes in female gonads LOEC: 170 µg TBT/kg dw Parasites (numbers of infected organisms) LOEC: 170 µg TBT/kg dw [all correspond to 190 at 5 % TOC] No effect of TBT exposure on survival or female sexual maturation. Unclear reagarding male sexual maturation. Frequency of dead oocytes increased significantly at TBT high conc. Significantly more parasite infected females in TBT high.	5 ± 0.5 °C	Klimish score: 2 Ecologically relevant study. Relevant for Swedish conditions. pH not reported. The study was carried out at a low temperature (5 °C). Only three TBT test concentrations, thus LOEC and NOEC may be under- and overestimated respectively. Some of the results are a bit ambiguous, and the statistical significance unclear. Relatively high level of organic content, which	Jacobson et al 2011

Organism	Method	Limnic / Marine	Organic carbon[1]; sediment type	Duration	Endpoint/s	Effect conc (µg TBT/kg dw)[2]	Physico-chemical conditions	Validity/relevance	Reference
	Measured concentrations Control: 13 ng TBT/g dw Low: 70 ng TBT/g dw High: 170 ng TBT/g dw							may lead to high effect concentrations.	
Echinocardium cordatum (both field and laboratory cultured organisms)	Control sediment was spiked with tributyltin (TBT) according to the method described by Bowmer (1993). In the 14 d whole sediment toxicity bioassay mortality was tested in a 750cm2 aquarium with a 10 cm layer of sediment and covered with 10 cm of filtered seawater with a salinity 32±4 g l−1. All tests with four replicates per treatment, each containing 10 organisms. Nominal concentrations: 0, 425, 852, 1705, 5253, 8542 and 17047 µg Sn/kg dry weight Measured concentrations (after 14 days exposure) Range from 9.6 to 16,646 µg Sn/kg dry weight (82 to 98 % of the nominal concentrations). Individual concentrations are not reported.	Marine	OC not reported Control sediment from Eastern Scheldt. Sediments from the port of Rotterdam, control sediments from clean site in Oesterput. Type of sediments not reported.	14 d	Survival (non-reburial activity)	Field *E. Cordatum*: LC50 = 702 ng Sn/g dw --> 1685 µg TBT/kg dw Cultured *E. Cordatum*: LC50 = 1525 ng Sn/g dw --> 3660 µg TBT/kg dw The results show that TBT is moderately toxic to the test organisms. It was also concluded that cultured heart urchins are less sensitive to TBT than field collected E. cordatum. In whole sediment toxicity tests, survival of cultured sea urchins was higher or at least similar to that of field collected E. cordatum.	15 ± 2 °C	Klimish score: 2 Generally, ecologically relevant study. However, only tested for mortality. Relevance to Swedish conditions could not be assessed. Several physico-chemical parameters are not reported, however there are references to older studies.	Schipper et al 2008
Hyalella azteca *Hexagenia limbata* (mayfly larva) *Physella gyrina* (pulmonate gastrophod)	The sediment was spiked with TBT chloride (Alfa Aesar) to a nominal conc of 5000 ng Sn/g, dilutions were prepared by adding control sediment. The experiments were conducted in 40 l glass aquaria containing a 9:1 ratio of overlying water to	Limnic	2 % TOC Sediments from Lake Erie (Canada), composed of 14 % sand, 49 % silt, 37 %	16 weeks	Growth, survival	H limbata: No effect on survival at low or intermediate conc, complete mortality at the highest conc. LOEC/LC100 = 1900 ng Sn/g --> 4560 µg TBT/kg dw [11 000 at 5 % TOC]	Mean pH was 8.3, range was 7.9 to 8.6. 25 ± 1 °C	Klimish score: 2 High temperature and pH, otherwise suitable for Swedish conditions. Several different species, but since	Bartlett et al 2007

Organism	Method	Limnic / Marine	Organic carbon[1]; sediment type	Duration	Endpoint/s	Effect conc (µg TBT/kg dw)[2]	Physico-chemical conditions	Validity/relevance	Reference
Tubifex tubifex (oligochaete) *Chironomus riparius* (midge larva) *Daphnia magna* (cladoceran) Freshwater invertebrates. The selection of species encompasses a range of life cycles, feeding habits and burrowing behaviours, all of which may modify toxicity.	sediment. All species were exposed simultaneously in each aquarium. There were 12 aquaria in total; 3 replicates/ concentration. Nominal concentrations: 0 ng Sn/g = ng TBT/g 50 ng Sn/g = ng TBT/g 500 ng Sn/g = ng TBT/g 5000 ng Sn/g = ng TBT/g The nominal concentration range was based on the results of previously conducted chronic toxicity tests with H. azteca, where no effects occured at 50 ng Sn/g and almost complete mortality occured at 5000 ng Sn/g. Measured test conc: below LOD 28,6 ng Sn/g = ng TBT/g 258 ng Sn/g = ng TBT/g 1900 ng Sn/g = ng TBT/g		clay and 2 % total organic carbon. Top 10 cm used in test. Density = 1.28 mg/L, moisture content = 54.2 %"			P. gyrina: No effect on the number of adult organisms at low or intermediate conc, significant drop in survival at the highest conc. (to 64 % of control values) Growth was not affected. LOEC = 1900 ng Sn/g --> 4560 µg TBT/kg dw [11 000 at 5 % TOC] H. azteca: No statistically significant effect. T tubifex: No effect at low or intermediate conc, complete mortality at the highest conc. LOEC/LC100 = 1900 ng Sn/g --> 4560 µg TBT/kg dw [11 000 at 5 % TOC] C. riparius: The toxicity of TBT could not be reliably quantified. No negative effects with increasing levels of TBT were detected, but survival was vey low in control aquaria (<15 %). D magna: No effect at low or intermediate conc, complete mortality at the highest conc. LOEC/LC100 = 1900 ng Sn/g --> 4560 µg TBT/kg dw [11 000 at 5 % TOC] The toxicity of TBT was similar in four out of six species of freshwater invertebrates. Statistically significant toxic effects were observed only at the highest TBT conc in H.		only three TBT conc. are tested, differences between the species is not easily detected in the test.	

Organism	Method	Limnic / Marine	Organic carbon[1]; sediment type	Duration	Endpoint/s	Effect conc (µg TBT/kg dw)[2]	Physico-chemical conditions	Validity/relevance	Reference
						limbata, P. gyrina, T. tubifex and D. magna, and there were no detectable effects on sublethal endpoints (i.e. growth, reproduction) in any of the test species at levels below those at which survival was affected.			
Hyalella azteca Cultured organisms, ref to Borgmann et al 1989. Young organisms (0-1 week old) were used for the toxicity test.	Experiments were conducted in 250 mL glass beakers containing 180 mL water and 20 mL sediment. Reference to Bartlett et al 2004b for information on conditions etc. Three replicates per sediment sample for each type of test. Test beakers were aerated through the experiments. Max conc in harbour sediments: Kingston: > 4000 ng Sn/g Montreal: > 800 mg Sn/g Port Weller: 520 ng Sn/g Toronto: 310 ng Sn/g Hamilton: < 100 ng Sn/g	Limnic	2 % TOC (in control sediments, harbour sediments not reported) Sediments from Canadian freshwater harbours historically contaminated with TBT; Montreal, Kingston, Toronto, Hamilton and Port Weller. Control sediments from Lake Erie , composed of 14 % sand, 49 % silt, 37 % clay and 2	4 weeks	Growth, survival	No observable effect of TBT on survival or growth; NOEC Kingston = > 4000 ng Sn/g = > 9600 µg TBT/kg dw [24000 at 5 % TCO] NOEC Montreal = > 800 mg Sn/g = > 1920 µg TBT/kg dw [4800 at 5 % TOC] NOEC Port Weller = 520 ng Sn/g = 1248 µg TBT/kg dw [3100 at 5 % TOC] NOEC Toronto = 310 ng Sn/g = 744 µg TBT/kg dw [1900 at 5 % TOC] NOEC Hamilton = 100 ng Sn/g = 240 µg TBT/kg dw [600 at 5 % TOC] (Results for spiked sediment is reported in Bartlett et al 2004, see below). In conclusion, TBT in Canadian freshwater harbours does not appear to be a major environmental concern. TBT in field	pH range was 7.9 to 8.6. 25 ± 1 °C	Klimish score: 2 High temperature and pH, otherwise suitable for Swedish conditions. High NOEC values, indicating that H azteca is not very sensitive (re growth/survival), which is supported by the results in Bartlett et al 2004, see below.	Bartlett et al 2005

Organism	Method	Limnic / Marine	Organic carbon[1]; sediment type	Duration	Endpoint/s	Effect conc (µg TBT/kg dw)[2]	Physico-chemical conditions	Validity/relevance	Reference
			% total organic carbon. Sediment type for the harbours not reported.			sediments was less bioavailable than in laboratory spiked sediments.			
Hyalella azteca Cultured freshwater amphipod invertebrates. Zero to one week old at the beginning of each experiment.	The chronic toxicity of TBT chloride (Alfa Aesar) was examined by exposing two successive generations of the freshwater amphipod Hyalella azteca to sediments spiked with TBT. Sediments were spiked to a nominal concentration of 9000 ng Sn/g DW, from which a series of TBT-spiked sediments ranging from nominal conc of 90 to 5000 ng Sn/g DW were made. The range of test concentrations was based on preliminary experiments that showed no effect on survival at nominal sediment conc of 90 ng Sn/g, and almost complete mortality at 5000 ng Sn/g. Sediment toxicity experiments were conducted in 250-ml glass beakers containing 180 ml of water and 20 ml of sediment. To initiate each experiment, 20 zero- to one-week-old animals were added to each beaker.	Limnic	TOC 2 % Sediments from Lake Erie (Canada), composed of 12 % sand, 49 % silt, 37 % clay and 2 % total organic carbon.	28 d 70 d	Survival, biomass production, reproduction	Survival: 4-week LC25 = 951 ng Sn/g dw = 2282 µg TBT/kg dw [5700 at 5 % TOC] 4-week LC50 = 1460 ng Sn/g dw = 3504 µg TBT/kg dw [8800 at 5 % TOC] 10-week LC25 = 533 ng Sn/g dw = 1279 µg TBT/kg dw [3200 at 5 % TOC] 10-week LC50 = 933 ng Sn/g dw = 2239 µg TBT/kg dw [5600 at 5 % TOC] Biomass production: 4-week EC25 = 1040 ng Sn/g dw = 2496 µg TBT/kg dw [6300 at 5 % TOC] 4-week EC50 = 1480 ng Sn/g dw = 3552 µg TBT/kg dw [8900 at 5 % TOC] 10-week EC25 = 1010 ng Sn/g dw = 2424 µg TBT/kg dw [6100 at 5 % TOC] 10-week EC50 = 1300 ng Sn/g dw = 3120 µg TBT/kg dw [7800 at 5 % TOC] Reproduction: 10-week EC50 = 238 ng Sn/g dw = 571 µg TBT/kg dw [1400 at 5 % TOC] No living young were produced between weeks 8	25 ± 1 °C pH 8.37	Klimish score: 2 High temperature and pH, otherwise suitable for Swedish conditions. Reproduction is the most sensitive endpoint. EC25 reported.	Bartlett et al 2004

Organism	Method	Limnic / Marine	Organic carbon[1]; sediment type	Duration	Endpoint/s	Effect conc (µg TBT/kg dw)[2]	Physico-chemical conditions	Validity/relevance	Reference
	The experiments were conducted twice with two replicates per concentration per experiment. Nominal concentrations: 90, 160, 280, 500, 900, 1600, 2800, 5000, and 9000 ng Sn/g dw Tributyltin levels measured in spiked sediment samples were approximately 50 % of nominal for all concentrations, except the highest, which was only 38 % of nominal					and 10 at nominal concentrations of 900, 5000, and 9000 ng Sn/g dw			
Potamopyrgus antipodarum (freshwater mudsnail). Specimens from laboratory breeding stock	Artificial sediments were spiked with seven nominal concentrations. Static test system (no water renewal) in 1-L glass flasks. Aerated sediments. 80 Potamopyrgus were added to each flask. A control and a solvent control was included in the test. Nominal TBT concentrations: 5, 10, 25, 50, 125, 250 and 500 µg Sn/kg dw (1 µg Sn corresponds to 2.44 µg TBT) Measured TBT concentrations (after eight weeks): 14.9, 20.1, 13.8, 70.6, 95.4, 152 and 396 µg Sn/kg dw	Limnic	TOC 2.3 % Spiked artifical sediments. 95 % quarts, 5 % grinded beech leves (for optimal embryo production) .	2, 4 and 8 weeks	Embryo production	Embryos without shell 4 weeks: EC10 = 0.98 µg Sn/kg = 2.4 µg TBT/kg [5.2 at 5 % TOC] EC50 = 45.8 µg Sn/kg = 110 µg TBT/kg [240 at 5 % TOC] Eight weeks: **EC10 = 2.98 µg Sn/kg = 7.2 µg TBT/kg [16 at 5 % TOC]** EC50 = 64 µg Sn/kg = 154 µg TBT/kg [330 at 5 % TOC] Total embryos 4 weeks: EC10 = 10.6 µg Sn/kg = 25.4 µg TBT/kg [55 at 5 % TOC] EC50 = 173 µg Sn/kg = 415 µg TBT/kg [900 at 5 % TOC] Eight weeks: EC10 = 3.5 µg Sn/kg = 8.4 µg TBT/kg [18 at 5 % TOC] EC50 = 93.9 µg Sn/kg = 225 µg TBT/kg [490 at 5 % TOC]	15±1 °C	Klimish score: 2 Relevant for Swedish conditions in terms of organic carbon, temperature and test species. However, pH not reported and artificial sediments. Low calculated effect concentrations. EC10 reported.	Duft et al 2003

Organism	Method	Limnic / Marine	Organic carbon[1]; sediment type	Duration	Endpoint/s	Effect conc (µg TBT/kg dw)[2]	Physico-chemical conditions	Validity/relevance	Reference
						LC50 (4 weeks) = 542 µg Sn/kg = 1301 µg TBT/kg [2800 at 5 %TOC] LC50 (8 weeks) = 431 µg Sn/kg = 1034 µg TBT/kg [2200 at 5 % TOC] LOEC (4 weeks) = 10 µg Sn/kg = 24 µg TBT/kg [52 at 5 % TOC] The number of unshelled embryos (the most sensitive parameter) decreased continously and significantly in all tested TBT conc and reached zero at the highest conc. EC10 for the eight week study was slightly higher than for the four week study which was unexpected.			
Armandia brevis A deposit-feeding Opheliid polychaete. Collected from sediments at Mitchell Bay, WA, USA, with no detected levels of TBT.	Sediments were spiked with a concentrated solution of TBT in acetone (100 mL sediment and 900 mL seawater in glass jars). Nine TBT treatments + controls. Sediments were analyzed on days 0, 21 and 42 to determine conc and check for loss of TBT. Range of measured sediment concentrations: 7 - 2556 ng TBT/g dw (mean of measures at day 21 and day 42)	Marine	0.6 % TOC Sediment from Mitchell Bay	21 d 42 d	Growth, survival	Growth: EC10 = 34 µg TBT/kg dw [280 at 5 % TOC] EC25 = 93 µg TBT/kg dw [770 at 5 % TOC] EC50 = 224 µg TBT/kg dw [1900 at 5 % TOC] Survival: LC50 = 902 µg TBT/kg dw [7500 at 5 % TOC] These results demonstrate that contaminant-induced sub lethal responses such as growth are more sensitive than mortality, and that juveniles appear to be more sensitive than adults. The sediment concentration (93 ng/g) causing a 25 %	13 ± 1 °C pH 8	Klimish score: 2 Very low organic carbon content, which indictes that the results may be conservative. EC10 reported.	Meador & Rice 2001

Organism	Method	Limnic / Marine	Organic carbon[1]; sediment type	Duration	Endpoint/s	Effect conc (µg TBT/kg dw)[2]	Physico-chemical conditions	Validity/relevance	Reference
						reduction in growth (EC25) for A. brevis is commonly exceeded in urban sediments. When normalized to organic carbon content, the day 42 LC50sedoc was 1.58E-5 ng TBT/g organic carbon in these exposures with juvenile A. brevis. The LC50sedoc can be used to determine the LC50sed for other sediments with differing amounts of organic carbon. For example, the LC50sed for a 1.5 % TOC sediment is predicted to be 2550 ng/g dry sediment.			
Echinocardium cordatum *Corophium volutator* Deposit feeders, limited knowledge on pathways of exposure. *E cordatum:* Adults of 3 - 6 cm, taken from an off-shore location in the north sea. *C volutator:* Adults collected from intertidal flat in the eastern Scheldt estuary.	Sediment samples were spiked by adding TBT chloride (Aldrich) to wet sediments. Toxicity test for E. cordatum were performed according to the Oslo and Paris Commission ring-test guideline. Flowing uncontaminated seawater. Each spiked sediment were tested in triplicate for mortality. 6 - 10 individuals per test. Tests for C. volutator were performed according to European Community Guidelines. Spiked sediments in 1-L glass jars, filtered seawater added, then aerated for 24 hours. Each test concentration was	Marine	TOC **2 %** Silty (fine) marine sediments, collected in the Rhine estuary. The spiked sediments were allowed to stand for 47 days to enable the TBT to reach equilibrium.	E cordatum: 28 d C. volutator: 10 d	Survival	E cordatum 14 d: NOEC = 1144 ng Sn/g dw = 2746 µg TBT/kg dw [6900 at 5 % TOC] LC50 = 4055 ng Sn/g dw = 9732 µg TBT/kg dw [24000 at 5 % TOC] E cordatum 28 d: NOEC = 1144 ng Sn/g dw = 2746 µg TBT/kg dw [6900 at 5 % TOC] LC50 = 1594 ng Sn/g dw = 3826 µg TBT/kg dw [9600 at 5 % TOC] C volutator 10 d: NOEC = 1144 ng Sn/g dw = 2746 µg TBT/kg dw [6900 at 5 % TOC] LC50 = 2185 ng Sn/g dw = 5244 µg TBT/kg dw [13000 at 5 % TOC]	E cordatum: 14 - 15.4 °C C. volutator: 14.8 - 15.8 °C pH: E cordatum: 7.5 - 8.1 C volutator: 8.1 - 8.3 pH sed: 7.7	Klimish score: 2 Relevant for Swedish conditions. The differences between NOEC and LC50 are rather small.	Stronkhorst et al 1999

Organism	Method	Limnic / Marine	Organic carbon[1]; sediment type	Duration	Endpoint/s	Effect conc (µg TBT/kg dw)[2]	Physico-chemical conditions	Validity/relevance	Reference
	tested in duplicate with 20 individuals per test. Concentration in sediment befor spiking: 17 ng Sn/g dw Nominal concentrations: 0, 32, 100, 320, 1000, 3200 and 10000 ng Sn/g dw Measured concentrations (after 28 days): 20, 24, 46, 179, 1144, 2383 and 11256 ng Sn/g dw					The bioavailability of TBT in the silty marine sediment is strongly reduced by sorption to organic matter and probably also to the large fraction of minerals present.			
Meiobenthic communities	Microcosms consisted of 570 mL glass bottles. Experimental sediment was amended with TBT chloride to achieve low, medium and high dose levels in experimental treatments. Spiked sediment was mixed in to the microcosms to achieve target TBT conc. There were four replicate microcosms for each TBT contaminated treatment and eight uncontaminated controls which were randomly located spatially within crates. Multivariate data analysis was done using non-metric multidimensional scaling ordination (MDS) with the Bray- Curtis similarity measure and using a range of transformations.	Marine	OC not reported. Three locations in SW England: Lyncher estuary (muddy sed) Exe estuary (sandy sed) Rame Head, Plymouth (muddy sand)	2 months	Number of species, abundance of nematode communities.	Lynher: Meiofauna (identified species/number of individuals) affected at the medium dose only. Exe: Significant effects at all three TBT conc (not measured, target conc was 0.3, 0.6, and 0.9 µg Sn/g dw = 0.7, 1.4 and 2.2 µg TBT/g dw). Rame Head: Significant effect at the highest dose. Effects were observed throughout the community (i.e. at all levels of data transformation) only at the highest TBT dose levels in the Exe estuary and Rame Head	20 °C	Klimish score: 2 Ecologically relevant study. Relevance for Swedish conditions could not be assessed since not all physico-chemical parameters are reported. Temperature relevant for summer conditions. Large focus on different types of statistical evaluation. Only three different TBT test concentrations; all rather high. No NOEC could be established for the	Austen & McEvoy 1997

Organism	Method	Limnic / Marine	Organic carbon[1]; sediment type	Duration	Endpoint/s	Effect conc (µg TBT/kg dw)[2]	Physico-chemical conditions	Validity/relevance	Reference
	Untransformed data analysis is more sensitive to changes in dominant species but increasingly severe square root and double square root transformations are more sensitive to changes in species composition. Hence analysis using different transformations provides an indication of which components of the community are being affected by the treatment, e.g. dominant and abundant species; common, slightly lower abundance species; and rare species. Target values: 0, 0.3, 0.6 and 0.9 µg Sn/g dw. Measured values: Lyncher estuary: 0.04, 0.27, 0.48 and 0.95 µg Sn/g dw. Rame Head: 0.01, 0.19, 0.53 and 0.92 µg Sn/g dw. Samples from Exe estuary were destroyed during storage before metal analysis could be carried out.					samples and (peculiarly) in the medium dose levels in the Lynher estuary. The Exe estuary fauna was also significantly affected by TBT at low and medium dose levels (when the data were transformed) and was therefore the most sensitive of the tested communities. Even though the treatment effects of some of the different dose levels were significant, the meiofaunal response was not one of large changes in community structure or gross mortality. There were almost no significant differences between treatments and controls in the univariate measures of nematode community structure. Mean numbers of species per microcosm averaged across all treatments were 22, 20 and 33 for Lynher, Exe and Rame Head samples, respectively, and the corresponding mean abundances were 3870, 910 and 590, respectively.		sandy sediment because there were effects at all tested conc. Differences in response due to type of sediment or to the meiobenthic communities, which could not be established.	

[1] If only the ”loss-on-ignition” (LOI) was stated in the publication, TOC was estimated by division with 1.724 (see ”Undersökningstyp Sediment – basundersökning”. https://www.havochvatten.se/download/18.64f5b3211343cffddb28000812/1348912814052/Sediment+-+basunders%C3%B6kning.pdf

[2] If results were expressed on the basis of the tin (Sn) content, it was converted to TBT content (by multiplication by 2.4). Values within parentheses is normalized to 5% OC (if possible) this was done by multiplying the effect value with 5 and then divided by actual TOC content.

8. SUPPORTIVE INFORMATION: Koc VALUES

Tabell S2. Koc values for TBT. Koc intervals used in calculations, based on the reliability and relevance for Swedish environmental conditions, are given in bold.

Method	Environment	TBT conc (water)	TBT conc (sediment)	Physico-chemical conditions	Koc and Kd	Conclusion in article	Validity/ Relevance	Reference
The partition coefficients were determined as conc ratios between sediment (K'd) or particulate (Kd) phase and dissolved phase of seawater. Koc was obtained by normalizing K'd for the organic carbon content in sediment.	19 sampling sites along the northeast mediterranean Spanish Coast(1988)	Enclosed vessel anchorages: 74 - 369 ng/l Commercial and fishing harbors: 14 - 30 ng/l	Max: 9260 ng/g	pH? Seawater TOC?	Koc? K'd values are reported in a plot; the range is between ca 500 - 100000.	The partion coefficients were one order of magnitude higer for triphenyltins than for butyltins. K'd for TBT is increasing with increased sediment concentrations.	Klimisch 3 The aim of the study was not to focus on partition coefficents. Too little information to make an assment of the relevance to Swedish conditions.	Tolosa et al 1992
Factorial experiments to investigate the effect of pH, particulate matter and salinity. For the estuarine experiments, 12 factorial experiments were undertaken in duplicate along with experimental blanks. Batch isoterm experiments to study the importance of concentration of particulate matter and sediment type in TBT sorption.	Sampling sites in the UK (sediment and water); Trowse Mill (sandy-silt) Rockland (silty-sand) Cantley (silty clay) (River Yare, Norfolk, UK) Water used in factorial experiments (uncontaminated with organotin compunds); Snape Quay (freswater) Orford Haven (saline) (Suffolk, UK)	TBT added to uncontaminated water and aqueous concentrations of TBT were calculated. TBT sorption isoterm data for freshwater sediments (µg/l): Cantley: 0.016 - 0.209 Rockland: 0.029 - 0.251 Trowse: 0.046 - 0.313	Sorbed sediment concentrations were found by difference relative to available TBT. TBT sorption isoterm data for freshwater sediments (µg): Cantley: 0.511-0.704 Rockland: 0.469 - 0.691 Trowse: 0.405 - 0.674	Trowse Mill: 1.4 % TOC; pH 7.6 Rockland: 12.5 % TOC; pH 7.2 Cantley: 6.9 % TOC; pH 7.8 TOC in sediment and interstitial water: 0.9 - 9.8 % (10 sites, mainly marinas and boatyards) Snape Quay: pH 7.95 Orford Haven: pH 7.93 Estuarine water experiments: pH 6 – 8	Koc? TBT sorption isoterm data for freshwater sediments (Kp): Cantley: 1464 - 4973 Rockland: 960 - 2493 Trowse: 398 - 896 Kp in sediment and interstitial water: 1.48E3 - 5.55E4 (10 sites, mainly marinas and boatyards)	TBT adsorption varied with sediment type, increasing in the order sandy silt < silty sand < silty clay. The TBT partition coefficient in interstial waters appears to be related to total organic carbon loadings.	Klimisch 2 No replicates. Batch isotherm experiments. Good distribution of TOC, values, overlaping the Swedish measured values.	Dowson et al 1993

Method	Environment	TBT conc (water)	TBT conc (sediment)	Physico-chemical conditions	Koc and Kd	Conclusion in article	Validity/ Relevance	Reference
				Water from Orford Haven was diluted to give salinity values of 5, 17.5 and 35 ppt.				
Batch testing methods using ^{14}C-TBT and natural sediment/water systems. For the K d determinations, two to five replicate treatments were used for each sediment. In the present study, the influence has been determined of some of the major parameters which affect the association of TBT with particulate material and its subsequent release, namely salinity, pH, suspended solids and sediment composition.	UK: Tamar Estuary Avon Estuary (for pH dependency) Poole Harbour Several other estuarine and coastal locations were used for the comparisons between sediment types.	the concentration of TBT in water covered a range of 6-6000 ng/l (as TBT) Summary statistics, mean values (ng/l as Sn): Poole 1985 -1988: 44.4 (n=24) Poole 1988-1990: 16.5 (n=29) Poole 1990-1992: 6.9 (n=39) Tamar 1991: 1.7 (n=0)	Summary statistics, mean values (µg/g as Sn): Poole 1985 -88: 0.16 Poole 1988-90: 0.14 Poole 1990-92: 0.1 Tamar 1991: 0.023	16 TOC values reported from different sites ranging from 1.32-11.7 % Salinity ranging from freshwater to full strength seawater (four replicates at each salinity) pH 4-10	Koc (Kd normalised with respect to the content of organic matter of sediments): 16 values reported from different sites ranging from 188 to 2814 16 Kd values reported from different sites, ranging from 248 to 24677 (each value reported is the calculated mean of four replicates) Summary statistics, based on mean values: Poole 1985 -88: 5170 Poole 1988-90: 10992 Poole 1990-92: 32969 Tamar 1991: 20798	Partitioning is influenced by salinity (lowest Kd values at low to intermediate salinities) and pH (highest Kd values occuring at neutral pH). Sediment characteristics also influenced partitioning; Kd were positively correlated with the concentration of total organic matter, humic substances, and high content of silt. The proportion of TBT bound 25 oparticles declined as the level of contamination increased.	Klimisch 2 Batch experiments, 2 – 5 replicates. Repeated sampling of selected sampling sites (Poole/Tamar). Based on available Swedish values what values for TOC, the most relevant Kd vales are 5102 and 8166. However, several other parameters are also important when assessing relevance.	Langston & Pope 1995
Sorption-desorption batch experiments using contaminated freshwater harbour sediments and two	Lake Zurich; Switzerland Harbor Wädenswil (sample ID W2) and Harbor Enge (E2).	In situ experiments (calculated average values from 13 vertical layers):	In Situ experiments (average observed values from 13 vertical layers)	No listed TOC values. Particulate organic carbon (POC) is listed	Laboratory experiment W2 - log Doc = 5.37 PACS-1 - log Doc =	At ambient pH values the sorption of triorganotins to sediments were dominated by complex formations of the	Klimisch 2 Duplicates of laboratory deteminition of Kd.	Berg et al 2001

Method	Environment	TBT conc (water)	TBT conc (sediment)	Physico-chemical conditions	Koc and Kd	Conclusion in article	Validity/ Relevance	Reference
certified OT containing marine sediments. The sediment-water distribution ratios determined in the laboratory were compared with *in situ* distribution ratios calculated from solid pore water concentration depth profiles.	Non natural "marine sediments"; PACS-1 and PACS-2 (two certified OT containing sediments).	W2 = 17 ng/l E2 = 9.8 ng/l	W2 = 350 ng/g E2 = 240 ng/g	for sediment and dissolved organic matter (DOC) for porewater. Porewater pH W2=7 E2=7.2 Lake water	5.46 PACS-2 - log Doc = 5.11 In situ experiments (calculated average values) W2 - log Doc = 5.69 E2 - log Doc = 5.73 Laboratory experiment W2 - log Kd = 4.13 PACS-1 - log Kd = 4.03 PACS-2 - log Kd =3.61 In Situ experiments (average observed values) W2 - log Kd = 4.34 E2 - log Kd = 4.39 (Kd = 21878 and 24547)	positively charged OT species with oxygen ligands present in the POM.	High TBT-levels in sediments, TOC not listed.	
Batch systems of 50 ml water phase and 1 g dried sediment in Erlenmeyer flasks were used. Sorption constants were calculated by regression analysis of isotherm equations. Experiments were conducted both in the field and in the laboratory.	Sediment samples from the vicinity (sea, esuary, river) of Haihe River, Tianjin, China S-1: Sea S-2: Estuary S-3: River Ambient natural water.	Ambient water: S-1: 62.9 ng Sn/L S-2: no data S-3: no data	S-1: 95.8 ng Sn/g S-2: no data S-3: no data	TOC S-1: 2.1 % S-2: 4.3 % S-3: 4.5 % Sediment pHs: 6.6 - 7.6 To dtermine the influence of pH on sorption, pH from 3 - 10 were maintained in the batch system.	Koc? Kd(L/kg) under natural aqueous conditions: S-1: 576,5 S-2: 2137,3 S-3: 3837,5 When water-phase salinity was elevated, sorption of TBT on S-2 and S-3 decreased greatly.	Kd values were pH dependent, with the highest sorption occurring under mildly acidic (pH 6) conditions. A second sorption peak was observed above pH 10. Further, sorption of TBT decreased as salinity increased.	Klimisch 2+ Thourough description of the method, but no replicates. Relevant for Swedish conditions. Limitid data on TBT concentrations in sediment and water.	Dai et al 2003

Method	Environment	TBT conc (water)	TBT conc (sediment)	Physico-chemical conditions	Koc and Kd	Conclusion in article	Validity/ Relevance	Reference
				Salinity S-1: 30.8 ‰ S-2: 22.6 ‰ S-3: 3 ‰				
TBT sorption to natural sediments in artificial seawater. Sorption isoterm equation calculations	Sediment samples (0 - 10 cm) from four different locations within the Moreton Bay, Southeast Queensland, Australia, designated MM, FS, CS and SP. Samples MM (mangrove forest), FS (mud flat) and CS (sand bank, low tide) were expected to be relatively pristine and sample SP was collected from a commercial marina. Artificial seawater was used.	Initial aqueous concentraions: Range of 50 - 500 µg/l (7 samples)	Determined by the difference between initial and equilibrium aqueous TBT concentrations.	TOC in sediments: MM: 4,8 % FS: 2,6 % CS: 0,3 % SP: 2,2 % pH in sediments: MM: 7,5 FS: 7,5 CS: 8 SP: 7,5 During the sorption experiments solution pH was maintained at 4, 6 and 8. Salinity 5 and 30 psu	Koc? Kd was determined for the four sediment samples under various artifical seawater salinity and pH condidtions. In general TBT sorption to the four contrasting sediment samples followed the order: MM: 172 - 5210 l/kg FS: 66-1220 l/kg SP: 21-65 l/kg CS: 6.1-24.7 l/kg The Kd values follow the order of organic C content in the sediment samples.	TBT sorption/desorption in natural sediments in artificial seawater can be strongly influenced by changes in pH and salinity. The observed behaviour can be rationalized by considering the contrasting sorptive behavior of the neutral (TBTOH, TBTCl) and cationic (TBT+) species at given pH/salinity conditions.	Klimisch 2 No replicates (except for some experiments with the SP sample). High TBT-levels in the artificial seawater.	Burton et al 2004
A batch technique was used to determine the partitioning of TBT between the solid and water phase (see Hoch et al. (2002)) Based on the linear adsorption isotherms of TBT to different	Two types of clay minerals were used; Wyoming Na-montmorillonite (sample SWy) and crystallized kaolinite (sample KGa) and quartz sand (sample Qz)	100–1000 ng (Sn)/ml	Not specified	The minerals were enriched with sorbed organic matter; end C-content of minerals as follows: KGa: 0,02 % Swy: 0,28 % Qz: 0,1 %	Koc? Kd (l/kg): KGa: 51 SWy: 89 Qz: 25 Kd´ (l/m^2): KGa: 5.07E-03 SWy: 2.79E-03 Qz: 8.04E-02	The study points to the importance of identifying and characterizing sorbents and envrionmental conditions in order to predict and model TBT distribution in natural systems. The results demonstrate that numerous	Klimisch 2 Triplicates of adsorption studies. Testing corresponding to Tier 1 in OECD 106. Replicates during the enrichment with sorbed organic matter.	Hoch & Schwesig 2004

Method	Environment	TBT conc (water)	TBT conc (sediment)	Physico-chemical conditions	Koc and Kd	Conclusion in article	Validity/ Relevance	Reference
types of minerals at pH 6, adsorption coefficients (Kd) were calculated.	No natural sediments were used.			Sediment pH: 4–9 Salinity 0 ‰ (deionised water) or 32 ‰ (artifical seawater)		environmental parameters influence the adsorption process of TBT. Examples of such parameters are solid/solution ratio, clay content, pH and salinity. The strongest adsorption was found at high particle concentrations (40–100 g/l), a large proportion of clay and a low salinity (0‰). The maximum of adsorption was always noted at a pH between 6 and 7. However, the strongest effect on TBT adsorption was found when introducing organic matter, either as particulate organic matter or as adsorbed organic matter, into the reaction system. TBT was found to adsorb more strongly to organic matter than to mineral phases. Addition of 5 % POM to the KGa sample showed a linear increase of Kd from 51 up to 2700 l/kg. *(The results are in significant contrast to Unger et al (1988), who did not find any correlation between the sorption coefficient of TBT and the amount of TOC (0.3–19.8 % TOC) in the sediment phase.)*	Very low TOC levels. No values of TBT concentrations in sediement reported. The study was conducted in order to inverstigate the result when changing certain parameters, and does not reflect actual environmental conditions.	

Method	Environment	TBT conc (water)	TBT conc (sediment)	Physico-chemical conditions	Koc and Kd	Conclusion in article	Validity/ Relevance	Reference
TBT in porewater samples and sediment extracts were quantified by gas chromatography–mass spectrometry (GC–MS)	Triplicate sediment cores were colected from a commercial marina located in southeast Queensland, Australia	0.05 - 2.35 µg/l	Total TBT concentrations ranged from 220 µg/kg - 8750 µg/kg	Organic carbon: 0.8–1.7 % (3.3 % at 0–2 cm depth) SedimentpH: 7.6–8.1 Added water: 5 Deionised water was used.	$\log D_{OC}$ = range from 3.88 to 5.61 log Kd, obs values ranged from 1.99 to 3.69 KD, Obs [l/kg] is an observed distribution coefficient describing the relationship between sorbed (mg/kg) and pore-water (mg/l) concentrations.	Values for the Butyltin Degradation Index (BDI) were larger than 1 at depths greater than 10 cm below the sediment/water column interface. This indicates that substantial TBT degradation has occurred in the sediments, and suggests that natural attenuation may be a viable sediment remediation strategy.	Klimisch 2 No replicates. Testing corresponding to Tier 1 in OECD 106. Low TOC concentrations, high levels of TBT in sediments makes the study less relevant with regard to Swedish conditions.	Burton et al 2005
The effect of contact time (1 and 84 days) on TBT desorption from sediment was examined by performing five sequential desorption steps. This involved shaking sediment with artificial seawater, followed by centrifugation and retention of the supernatant. This procedure was repeated five times to simulate TBT desorption during repeated sediment resuspension events.	Three natural sediment samples (designated MM, FS and CS) were collected from the 0 - 5 cm depth interval at a low tide in Moreton Bay, Southeast Queensland, Australia.	Pore-water TBT (µg/l). 1 - 84 days, 7 samples. Sample CS: 15500 - 21400 Sample FS: 34 - 92.8 Sample MM: 11.3 - 21.4 The pore-water TBT concentrations observed in CS did not vary systematically as a function of contact time, but for samples FS and MM the porewater TBT concentrations for contact times of 1 day were greater than those for 84 days.	Sorbed TBT (µg/kg). 1 - 84 days, 7 samples. Sample CS: 3705 - 5244 Sample FS: 9964 - 9986 Sample MM: 9978 - 9988 Sorbed TBT was calculated by subtracting pore-water TBT from added TBT.	Sed (org C): CS: 0,2 % FS: 2,6 % MM: 4,8 % pH CS: 8 FS: 7,5 MM: 7,5 Artifical seawater, prepared according to Eckber gand Hill, no salinity reported in the article.	Koc? Kd, apparent (l/kg) Sample CS 0.18 - 0.34 Sample FS 107 - 286 Sample MM 466 – 687 *An apparent distribution coefficient is equal to the partition coefficient * fraction of the substance that is not ionised.*	Whilst short-term laboratory-based studies provide an improved understanding of the TBT sorption process, they may underestimate TBT binding to some natural sediments over longer time scales. This underestimation may lead to perceived requirements for sediment remediation in areas that pose little environmental risk and thereby divert funds from remediation projects where the risk is greater. The present study shows that aging may be an important consideration in TBT fate and is a subject warranting further research.	Klimisch 2- No replicates. 3 different types of sediment. Too high TBT-concentrations in sediment samples for Swedish conditions. Relevant TOC-levels in two of the locations (FS, MM).	Burton et al 2006

Method	Environment	TBT conc (water)	TBT conc (sediment)	Physico-chemical conditions	Koc and Kd	Conclusion in article	Validity/ Relevance	Reference
Kd values of TBT were determined by ASTM standard E1195-01 to measure TBT adsorption behavior (ASTM, 2001). The Kd value in the current study was obtained from the intercept of a log plot of the Freundlich equation to improve the correlation coefficient and assess the actual adsorption behavior of TBT.	Scotland, UK: Bowling basin (BB), Port Dundas (PD)and Clyde River (CR))	The concentrations of TBT in water were 40, 80, 120, 160, 200, 240 and 300 µg/mL.	Analyzed, but not specified in the article.	Sediment TOC BB: 12 % PD: 17 % CR: 1,2 % pH 4, 5, 6, 7 and 8 0, 15, 32, 50 and 100 psu	Koc? log Kd: BB: 3,64 *(4365)* PD: 3,48 *(3020)* CR: 1,95 *(89)* 89 to 4909 L/kg depending on sediment properties, salinity, pH, and temperature.	The Kd values depended on the following: (i) Organic carbon and clay mineral content which affected the sorption behavior (the lower the organic carbon, the lower the Kd). (ii) Salinity. The sorption was highest in freshwater and decreased at low and intermediate salinities indicating that bioavailability is higher in marine environments. At very high salinities, not typically experienced in the environment (100 psu), the Kd increased again. (iii) pH, the highest TBT adsorption of this study was at pH7 due to the charge contained on clay surfaces and dominant species of TBT. (iv) Temperature, the adsorption of TBT on sediment slightly increases at higher temperature due to the reduction	Klimisch 2 No replicates. Testing corresponding to Tier 1 in OECD 106 with Freundlisch evaluation. TOC concentrations not applicable for Swedish conditions. TBT concentrations in sediment were not specified.	Bangkedphol et al 2009a
Kd values of TBT were determined by ASTM standard E1195-01 to measure TBT adsorption behavior (ASTM, 2001). The method was developed by the author.	Scotland, UK: Bowling basin (BB) and Port Dundas (PD)	BB: 0.85 ±4.81 ppb PD: 0.17±1.72 ppb	BB: 162.31 ±0.13 ppb, PD: 148.89±0.51 ppb	Sediment BB: 12 % PD: 17 % pH BB: 8 PD: 8 Freshwater	logKoc, calculated from Kd: BB: 4.55 PD: 4.24 (Default value from EPI Suite V.3.20 was 4.18)	The comparison between values obtained experimentally and computated default model values (EPI Suite V. 3.20) differed. Koc values were higher than predicted, i.e. adsorption was stronger.	Klimisch 2- Simple model, no replicates. The aim of the model is to be simple. Too high TOC levels for Swedish conditions	Bangkedphol et al 2009b

Method	Environment	TBT conc (water)	TBT conc (sediment)	Physico-chemical conditions	Koc and Kd	Conclusion in article	Validity/ Relevance	Reference
					log Kd: BB: 3,63 *(4266)* PD: 3,48 *(3020)*			
Content of butyltins in water and sediments were determined by reflux extraction and Kd values by using sorption isoterms (Freundlish equation)	Oslo Harbour (low TBT) Drammen (high TBT)	1-2000 µg/l (artifical seawater)	Oslo: 3.7 µg/kg DW Drammen: 4300 µg/kg DW	TOC Oslo: 1.98 % Drammen: 3.7 % pH adjusted to around 8 (marine conditions) Artifical seawater, prepared according to Eckber gand Hill, no salinity reported in the article.	**log K_{TOC} Oslo: 4.6 - 5.3 (L/kg_{toc})** log K_{TOC} Drammen: 5.5 (L/kg_{toc}) log Kd Oslo: 3.1 - 3.6 log Kd Drammen: 4.07	The black carbon and TOC sorption results showed that sorption to black carbon does not need to be considererd in TBT fate modeling. Further sthe study indicates that powdered active carbon (AC) may be a feasible remediation agent, since AC was found to strongly sorb TBT under marine conditions.	Klimisch 2+ No replicates. Testing corresponding to Tier 1 in OECD 106 with Freundlisch evaluation. Relevant for Swedish conditions	Brändli et al 2009
Granulometric analyses of sediments and thermogravimetric analysis accompanied by chemical analyses of water and sediments were performed (determination of organotin, carbon, nitrogen and sulfur, pH and salinity). The average values listed are based on 8 samples. The listed values are average values.	Water and sediment from the most contaminated quays in the portof Gdynia	Feb: 118.6 ng cation/l June: 46.5 ng cation/l Note: the table in the article is skew.	Feb, fine fraction: 4400 ng cation/g June, fine fraction: 3638 ng cation/g June, coarse fraction (whole sediment): 2805ng cation/g	Sediment Feb, fine fraction: 7.9 % June, Fine fraction: 7.2 % June, coarse fraction (whole sediment): 4.3 % Water pH Feb: 7.4 June: 7.7 Water Feb: 8.05 PSU June: 8.05 PSU	Koc? Concentrations of TBT in water and sediments during different conditions reported, but no calculation of sorption coefficients.	The drop in butyltin concentrations in the period from February to June was very high, especially for the sediment samples. This can be explained by higher photodegradation and possibly biodegradation rates and by a more alkaline pH in June which influenced desorption of BT from sediments to the water column.	Klimisch 2 No replicates. Testing corresponding to Tier 1 in OECD 106 Too high TBT concentrations in sediment samples for Swedish conditions. Levels of TOC, pH and salinity are relevant.	Radke et al 2013

9. SUPPORTIVE INFORMATION: EqP CALCULATIONS

Calculations were based on equations and the default values given in European Communities (2011).

$$Kp_{\mathrm{sed}} = Foc_{\mathrm{sed}} \times K_{\mathrm{oc}} \quad (1)$$

$$K_{\mathrm{air-water}} = \frac{H}{R \times TEMP} \quad (2)$$

$$K_{\mathrm{sed\text{-}water}} = F\mathrm{air}_{\mathrm{sed}} \times K_{\mathrm{air-water}} + F\mathrm{water}_{\mathrm{sed}} + F\mathrm{solid}_{\mathrm{sed}} \times \frac{Kp_{\mathrm{sed}}}{1000} \times RHO\mathrm{solid} \quad (3)$$

$$QS_{\mathrm{sediment,EqP,ww}} = \frac{K_{\mathrm{sed-water}}}{RHO_{\mathrm{sed}}} \times QS_{\mathrm{fw,\ eco}} \times 1000 \quad (4)$$

$$CONV\mathrm{sed} = \frac{RHO_{\mathrm{sed}}}{F\mathrm{solid}_{\mathrm{sed}} \times RHO\mathrm{solid}} \quad (5)$$

$$QS_{\mathrm{sediment,EqP,dw}} = CONV\mathrm{sed} \times QS_{\mathrm{sediment,EqP,ww}} \quad (6)$$

Parameter	Description	Unit	Default value
1000	conversion factor from m^3 to litre	$L\ m^{-3}$	1000
$Cporew_{sed}$	total concentration in pore water of sediment	$mg\ m^{-3}$	
$Ctotal_{sed}$	total concentration in sediment	$mg\ m^{-3}$	
$Fair_{sed}$	fraction air in sediment	$m^3\ m^{-3}$	0
Foc_{sed}	weight fraction of organic carbon in sediment	$kg\ kg^{-1}$	0.05
$Fsolid_{sed}$	fraction solids in sediment	–	0.2
$Fwater_{sed}$	fraction water in sediment	$m^3\ m^{-3}$	0.8
H	Henry's law constant	$Pa\ m^3\ mol^{-1}$	
$K_{air\text{-}water}$	air-water partition coefficient	$m^3\ m^{-3}$	
K_{oc}	partition coefficient between organic carbon and water	$L\ kg^{-1}$	
Kp_{sed}	partition coefficient solid-water in sediment	$L\ kg^{-1}$	
$K_{sed\text{-}water}$	partition coefficient between sediment and water	$m^3\ m^{-3}$	
R	gas constant	$Pa\ m^3\ mol^{-1}\ K^{-1}$	8.314
RHO_{sed}	bulk density of wet sediment	$kg_{ww}\ m^{-3}$	1300
RHOsolid	density of the solid phase	$kg_{solid}\ m_{solid}^{-3}$	2500
$TEMP$	environmental temperature	K	285
$CONV$sed	conversion factor for sediment concentration wet-dry weight sediment	$kg_{ww} \cdot kg_{dw}^{-1}$	
$QS_{sediment,\ EqP,\ dw}$	dry weight quality standard for sediment based on equilibrium partitioning	$mg\ kg_{dw}^{-1}$	
$QS_{sediment,\ EqP,\ ww}$	wet weight quality standard for sediment based on equilibrium partitioning	$mg\ kg_{ww}^{-1}$	
$QS_{fw,\ eco}$	quality standard for direct ecotoxicity on freshwater aquatic organisms	$mg\ L^{-1}$	

9.1 Calculations

Values in bold indicates that these values are influenced if using another Koc.

$$Kp_{sed} = Foc_{sed} \times K_{oc} \qquad (1)$$

$= 0.05 \times \mathbf{40000} = \underline{2000}$

$$K_{air-water} = \frac{H}{R \times TEMP} \qquad (2)$$

Equation 2 not calculated since the first product of the equation 3 will be zero based on the default value specified for fraction air in the sediment ($Fair_{sed}$) which means that $Fair_{sed}$ x $K_{air-water}$ will be equal to 0 regardless of value calculated for $K_{air-water}$.

$$K_{sed\text{-}water} = Fair_{sed} \times K_{air-water} + Fwater_{sed} + Fsolid_{sed} \times \frac{Kp_{sed}}{1000} \times RHOsolid \qquad (3)$$

*= 0 + 0.8 + 0.2 x [**2000** /1000] x 2500=*<u>*1000.8*</u>

$$QS_{\text{sediment,EqP,ww}} = \frac{K_{\text{sed-water}}}{RHO_{\text{sed}}} \times QS_{\text{fw, eco}} \times 1000 \qquad 4$$

*= [**1000.8** /1300] x 0.0000002 x 1000 =*<u>*0.000154*</u>

$$CONV\text{sed} = \frac{RHO_{\text{sed}}}{F\text{solid}_{\text{sed}} \times RHO\text{solid}} \qquad 5$$

= 1300 /[0.2 x 2500] =<u>*2.6*</u>

$$QS_{\text{sediment,EqP,dw}} = CONV\text{sed} \times QS_{\text{sediment,EqP,ww}} \qquad 6$$

*= 2.6 x **0.000154=*** 0.0004 (mg/kg) – EqP QS of 0.4 µg/kg dw, at 5 % TOC

When LogKow is greater than 5 the calculated EqP QS should be divided by an AF of 10 to take into account uncertainties regarding uptake through diet. In the case of TBT, the LogKow was below 5 (varying between 3.1 and 4.1 according to the substance data sheet), hence, a AF was not required.

Parameter	Value used in the calculation	Unit	Comment
$F\text{air}_{\text{sed}}$	0	$m^3\ m^{-3}$	*Default*
$F\text{oc}_{\text{sed}}$	0.05	$kg\ kg^{-1}$	*Default*
$F\text{solid}_{\text{sed}}$	0.2	–	*Default*
$F\text{water}_{\text{sed}}$	0.8	$m^3\ m^{-3}$	*Default*
K_{oc}	**40000**	$L\ kg^{-1}$	
$K\text{p}_{\text{sed}}$	2000	$L\ kg^{-1}$	Based on equation 1
$K_{\text{sed-water}}$	1000.8	$m^3\ m^{-3}$	Based on equation 3
R	8.314	$Pa\ m^3\ mol^{-1}\ K^{-1}$	*Default*
RHO_{sed}	1300	$kg_{ww}\ m^{-3}$	*Default*
$RHO\text{solid}$	2500	$kg_{solid}\ m_{solid}^{-3}$	*Default*
TEMP	285	K	*Default*
$CONV\text{sed}$	2.6	$kg_{ww} \cdot kg_{dw}^{-1}$	Based on equation 6
$QS_{\text{sediment, EqP, ww}}$	**0.000154**	$mg\ kg_{ww}^{-1}$	Based on equation 5
$QS_{\text{fw, eco}}$	0.0000002	$mg\ L^{-1}$	EQS of 0,0002 µg/l = 0,0000002 mg/l according to 2008/105/EG.

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