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Schweizerisches Zentrum für angewandte Ökotoxikologie
Centre Suisse d'écotoxicologie appliquée

SQC (EQS_{sed}) – Proposal by the Ecotox Centre for: *Triclosan*

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Authors

Carmen Casado-Martinez, Swiss Centre for Applied Ecotoxicology

Scientific Support

Dr Karen Duis, ECT Oekotoxikologie GmbH, Böttgerstr. 2-14, D-65439 Flörsheim/Main, Germany. External reviewer.

Dean Leverett, Adam Peters, Becky Marks, Graham Merrington wca environment Ltd, Faringdon, Oxfordshire, SN7 7YR, UK. Scientific support on EQS derivation.

Please note that the suggested EQS and contents of this dossier do not necessarily reflect the opinion of the external reviewer.

Contact

Carmen Casado: carmen.casado@centreecotox.ch

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Oekotoxzentrum | Eawag | Überlandstrasse 133 | 8600 Dübendorf | Schweiz
T +41 (0)58 765 55 62 | info@oekotoxzentrum.ch | www.oekotoxzentrum.ch

Centre Ecotox | EPFL-ENAC-IIE-GE | Station 2 | CH-1015 Lausanne | Suisse
T +41 (0)21 693 62 58 | info@centreecotox.ch | www.centreecotox.ch



Summary

SQC (EQS_{sed}): 67.4 $\mu\text{g}/\text{kg d.w.}$

In the framework of the Module Sediment, which is intended to help cantons in sediment quality assessment, the Ecotox Centre develops proposals for Environmental Quality Criteria for sediment (SQC). SQC are derived applying the methodology described in the EU-Technical Guidance (TGD) for Deriving Environmental Quality Standards (EQS). In order to ensure that the dossiers are internationally comparable, the English terminology of the TGD will be used in the remainder of the dossier. These criteria provide a first screening tool to evaluate sediment chemical quality and the potential risk for the aquatic ecosystem. Based on the scientific literature available at present a preliminary SQC for triclosan of 67.4 $\mu\text{g}/\text{kg d.w.}$ is proposed for standard sediments with 1 % OC.

Zusammenfassung

SQK (EQS_{sed}): 67.4 $\mu\text{g}/\text{kg TS}$

Im Rahmen des Sedimentmoduls, das den Kantonen bei der Bewertung der Sedimentqualität helfen soll, entwickelt das Oekotoxzentrum Vorschläge für Umweltqualitätskriterien für Sedimente (SQK). Diese Kriterien dienen als Methode für ein erstes Screening zur Bewertung der chemischen Sedimentqualität und des potenziellen Risikos für aquatische Ökosysteme. Auf der Basis von Literaturdaten für die Wirkung von Triclosan und unter Verwendung der Methode, die in der Technischen Richtlinie der EU zur Ableitung von Umweltqualitätsnormen beschrieben wird, schlägt das Oekotoxzentrum einen vorläufiger SQK für Triclosan von 67.4 $\mu\text{g}/\text{kg TS}$ für Standardsedimente mit 1 % OC vor.

Résumé

CQS (EQS_{sed}): 67,4 $\mu\text{g}/\text{kg p.s.}$

Dans le cadre du module Sédiments qui devrait aider les cantons à évaluer la qualité des sédiments, le Centre Ecotox élabore des propositions de critères de qualité environnementale pour les sédiments (CQS). Les CQS sont dérivés en appliquant la méthodologie décrite dans le Guide Technique de l'UE (TGD) pour la Dérivation des Normes de Qualité Environnementale (EQS). Afin que les dossiers soient comparables au niveau international, la terminologie anglaise du TGD est utilisée ci-dessous. Ces critères fournissent un premier outil de dépistage pour évaluer la qualité chimique des sédiments et le risque potentiel pour l'écosystème aquatique. Sur la base des données sur les effets existants dans la littérature un CQS préliminaire pour le triclosan de 67,4 $\mu\text{g}/\text{kg p.s.}$ est proposé pour les sédiments standards avec 1 % CO.



Sommario

CQS: 67,4 µg/kg p.s.

Nell'ambito del modulo Sedimenti, che è finalizzato ad aiutare i Cantoni nella valutazione della qualità dei sedimenti, il Centro Ecotox sviluppa proposte per i criteri di qualità ambientale per i sedimenti (CQS). I CQS sono derivati applicando la metodologia descritta nella Guida Tecnica dell'UE (TGD) per la Derivazione degli Standard di Qualità Ambientale (EQS). Per garantire che i dossier siano comparabili a livello internazionale, viene utilizzata la terminologia inglese del TGD. Questi criteri forniscono un primo strumento di screening per valutare la qualità chimica dei sedimenti e il potenziale rischio per l'ecosistema acquatico. Sulla base della letteratura scientifica disponibile allo stato attuale un CQS preliminare per il triclosan di 67,4 µg/kg p.s. è proposto per sedimenti standard con 1 % CO.



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1 General Information

Selected information on the substance triclosan relevant for sediment is presented in this chapter. Registration information and risk assessments referred to are:

- EQS - Vorschlag des Oekotoxenzentrums für: Triclosan. Oekotoxzentrum 2017.
- Schlich K, Wenzel A, Shemotyuk L. EQS datasheet Triclosan. Fraunhofer Institute for Molecular Biology and Applied Ecology (IME) Auf dem Aberg 1 57392 Schmallingenberg Germany. On behalf of the Federal Environment Agency (Umweltbundesamt, UBA) Wörlitzer Platz 1 06844 Dessau-Roßlau Germany. May 2014.
- INERIS (2012): Normes de qualité environnemental triclosan– n° CAS: 3380-34-5. <https://substances.ineris.fr/fr/substance/2723>
- ECHA (2016) Information on Registered Substances: Triclosan, CAS number: 3380-34-5 <https://echa.europa.eu/registration-dossier/-/registered-dossier/12675/1> Last modified: 21-Sep-2016.
- Priority Existing Chemical Assessment Report No. 30: Triclosan. National Industrial Chemicals Notification and Assessment Scheme (NICNAS). January 2009. Commonwealth of Australia 2009 ISBN 0-9803124-4-2
- 5-chloro-2-(2,4-dichlorophenoxy) phenol (triclosan): Risk assessment for the Reregistration Eligibility Decision (RED) Document. Case No 2340. PC Code: 054901, April 17, 2008. Reregistration Eligibility Decision (RED) Document for Triclosan September 18, 2008. US Environmental Protection Agency.

1.1 Identity and physico-chemical properties

Triclosan is the most common name for 5-chloro-2-(2,4-dichlorophenoxy)phenol, a chlorinated aromatic compound with both phenolic and ether structural moieties which has been sold under several commercial names (e.g. Irgasan).

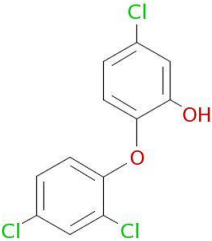
The log K_{oc} reported for triclosan are in the range of 3.90-5.26 (Table 1; geometric mean = 4.51, Appendix 1). Reported log K_{ow} range from 4.7 to 4.9 (Table 1). Both parameters trigger an effects assessment for sediments according to the EC TGD EQS (EC 2018).

Table 1 summarizes identity and physico-chemical parameters for triclosan required for EQS derivation according to the TGD (EC 2018). Where available, experimentally collected data is identified as (exp.) and estimated data as (est.). When not identified, no indication is available in the cited literature.

Due to limited time, primary references for physico-chemical properties as reported in cited reports/publications have not been verified and only secondary references are indicated for such data. These primary references are not included in the reference list, the reader is referred to the secondary report/publication.



Table 1 Information required for EQS derivation according to the TGD (EC 2018). Grey data are not used in EQS derivation (see text for details).

| Characteristics | Values | References |
|--|---|--|
| Common name | Triclosan | |
| IUPAC name | 5-chloro-2-(2,4-dichlorophenoxy)phenol | ECHA (2016) |
| Chemical group | Phenol | |
| Structural formula |  | ECHA (2016) |
| Molecular formula | C ₁₂ H ₇ Cl ₃ O ₂ | ECHA (2016) |
| CAS | 3380-34-5 | ECHA (2016) |
| EC Number | 222-182-2 | ECHA (2016) |
| SMILES code | <chem>C1=CC(=C(C=C1Cl)O)OC2=C(C=C(C=C2)Cl)Cl</chem> | ECHA (2016) |
| Molecular weight [g/mol] | 289.5 | PubChem (2020) |
| Melting point [°C] | [1] 56.4 (exp.) [2] 136.79 (est.) | [1] ECHA (2016) [2] EPI Suite™ (US EPA 2008) ¹ |
| Boiling point [°C] | [1] 120 °C [2] 280 to 290 °C (decomposes) [3] 373.62 (est.) | [1] PubChem (2020) [2] Fiege et al. (2000) cited in PubChem (2020) [3] EPI Suite™ (US EPA 2008) ¹ |
| Vapour pressure [Pa] | [1] 0.0003 Pa at 20 °C, 0.0007 Pa at 25 °C (exp. extrapolated) [2] 0.00062 (est.) | [1] ECHA (2016) [2] EPI Suite™ (US EPA 2008) ¹ |
| Henry's law constant [Pa·m ³ ·mol ⁻¹] | [1] 0.001 [2] 5.05*10 ⁻⁴ (est. Bond Method); 2.16*10 ⁻³ (est. Group Method) | [1] ECHA (2016) [2] EPI Suite™ (US EPA 2008) ¹ |
| Water solubility [mg·l ⁻¹] | [1] 3.6 (10 °C pH 5); 6.5 (20 °C pH 5); 10.8 (30 °C pH 5) [2] 10 (exp) | [1] ECHA (2016) [2] EPI Suite™ (US EPA 2008) ¹ |
| Dissociation constant (pK _a) | [1] 8.14 (20 °C) (exp.) [2] 8.01 | [1] ECHA (2016) [2] Sparc (2010) ¹ |
| Octanol-water partition coefficient (log K _{ow}) | [1] 4.8 (exp. OECD 107 shake flask method; 25 °C, pH 6.7) [2] 4.9 (calculated from the solubility in water and in n-octanol; range 4.7-5.2 10-30 °C, pH 5) [3] 4.76 (25 °C) [4] 4.76 (25 °C) | [1] ECHA (2016) [2] ECHA (2016) [3] NITE (1992) cited in ECHA (2016) [4] SRC (2009) cited in ECHA (2016) |
| Sediment/soil-water partition coefficient (log K _{oc}) | [1] 2.92 (exp. OECD 121 HPLC method) [2] 2.62 (exp. OECD 121 HPLC method) | [1-3] ECHA (2016) |



| Characteristics | Values | References |
|---|--|--|
| | [3] 4.68 (exp. US EPA 3.08 Batch equilibrium method; activated sludge 45.4 % OC) [4] 4.54 (exp. field study, freshwater sed., n=16) [5] 4.8 (exp. field study, freshwater sed., n=94) [6] 4.95, 4.90, 5.41 (exp. batch simulation study, freshwater sed.) [7] 4.17, 4.61 (exp. OECD 106 batch equilibrium study, freshwater sed., 1.0, 3.5 % OC) [8] 4.22 (exp. OECD 106 batch equilibrium study, freshwater sediment, OC 4.09 % Clay 60.5 % pH 7.9) [9] 4.17, 4.46, 5.26 (exp. batch equilibrium study, freshwater sed., 1.4, 1.9 and 2.3 % OC) [10] 3.90 (exp. batch equilibrium study, freshwater sed., 0.5 % OC) [11] 3.90 (est. from K_{ow}) | [4] Wang and Kelly (2017) [5] Zhao et al. (2013) [6] Lin et al. (2011) [7] Recalculated from Huang et al. (2014) [8] Recalculated from Huang et al. (2014); Wu et al. (2015) [9] Styszko (2016) [10] dos Santos et al. (2018) [11] Appendix 1 |
| Sediment adsorption coefficient (K_d [L/kg]) | [1] 1272 (exp. batch simulation study, freshwater sed., OM 2.44 % Clay 26.4 % pH 6.8) [2] 1393 (exp. batch simulation study, freshwater sediment, OM 2.97 % Clay 19.5 % pH 6.8) [3] 1572 (exp. batch simulation study, freshwater sediment, OM 1.05 % Clay 13.3 % pH 6.8) [4] 203 (exp. batch equilibrium study, freshwater sediment, OC 1.37 pH 7.7 Clay 7.0 %) [5] 531 (exp. batch equilibrium study, freshwater sediment, OC 1.83 pH 7.6 Clay 8.5 %) [6] 1144 (exp. batch equilibrium study, freshwater sediment, OC 2.03 pH 7.6 Clay 18.2 %) [7] 837 (geomean) [8] (exp. field study, estuarine sediment and SPM, average n=6) | [1-3] Lin et al. (2011) [4-6] Styszko (2016) [7] Appendix I [8] Wilson et al. (2009) |
| Aqueous hydrolysis DT_{50} | [1] > 1 y (exp. 25 °C pH 4-9) [2] Stable (exp. 50 °C pH 4-9) | [1] ECHA (2016) [2] US EPA 2008 cited in Schlich et al. (2014) |
| Aqueous photolysis DT_{50} | [1] 41 min (exp. 24.6-25.8 °C) [2] < 10 d | [1,2] ECHA (2016) |



| Characteristics | Values | References |
|--|--|--|
| Biodegradation in water-sediment systems DT_{50} [d] | 1.2 in river water and 56.4 in river sediment (exp. laboratory; OECD 308; 41.1 d in total system) 1.4 in pond water and 56.3 in pond sediment (exp. laboratory; OECD 308; 58.3 d in total system) | ECHA (2016) |
| Biodegradation in soil DT_{50} [d] | [1] 35.2 (silt loam), 29.1 (loam), 14.7 (sandy loam) (exp. laboratory; OECD 307); [2] 3.27 (clay loam, 20 °C), 10.7 (clay loam, 10 °C), 2.46 (sandy loam, 20 °C), 2.68 (20 °C) | [1] Colgate-Palmolive Company (1994) cited in ECHA (2016) [2] ECHA (2016) |

¹ Information gathered from Oekotoxzentrum (2017).

1.2 Regulatory context and environmental limits

The first US patent for triclosan was in 1964 (Merck 1983) and triclosan has been marketed for over 40 years (NICNAS 2009). The chemical was listed on the Organisation for Economic Cooperation and Development's (OECD) High Production Volume Chemicals list in 2004 (OECD 2004) and sponsored through the OECD SIDS program by Australia (NICNAS 2009; OECD 2009).

Triclosan was listed in the Prior Informed Consent (PIC) circular LI (51) – June 2020 of the Rotterdam Convention according to the regulation of triclosan in the EU. The Convention enables listed hazardous chemicals to be monitored and their trade controlled on a global scale. Triclosan is listed in Part 1 of Annex I and is therefore subject to the export notification procedure and in Part 2 of Annex I, in addition to being subject to export notification procedure, qualifying also for the PIC notification procedure as from 6 February 2018 (ECHA 2021).

Triclosan was pre-registered in 2010 but no full registration has been submitted as of 01 December 2020 (ECHA 2021). It is under assessment as Persistent, Bioaccumulative and Toxic and under assessment as Endocrine Disrupting (ECHA 2021).

According to toxicological information in ECHA (2016), triclosan is not classified for acute toxicity, mutagenicity, carcinogenicity and reproduction toxicity according to the Annex VI of the EU CLP regulation.

Triclosan is not included in the list of approved active substances under regulation (EU) No 528/2012. Therefore, as governed by Article 89(2)(b) it is prohibited to place on the market as of 17 February 2017 and to use as of 17 August 2017 biocidal products of product-type 1, human hygiene biocidal products, containing triclosan due to risks to the environment. Based on the consumption-based approach, a risk was identified for both surface water and for the non-compartment specific effects relevant to the food chain (secondary poisoning to birds, which appear more sensitive than mammals). Based on the specific evaluated use no possibilities for any risk mitigation measures seem to be realistic. Triclosan is also not approved for product-type 2, disinfectants and algacides not intended for direct application to humans or animals, product type-7, film preservatives and product type-9, fibre, leather, rubber and polymerised materials preservatives (decision 2014/227/EU). Switzerland adopts the assessment procedures for biocidal active substances from the EU. Accordingly, the same restrictions apply in Switzerland (Ordinance on Biocidal Products (OBP - SR 813.12))



Table 2 Existing regulation for triclosan in Switzerland and Europe.

| Europe | |
|--|--|
| EU Priority substance list | Not listed |
| EU Community Rolling Action Plan | Listed (EC 2020) |
| Biocides | Banned for - Product-type 1, human hygiene biocidal products (decision 2016/110/EU) - Product-type 2, disinfectants and algacides not intended for direct application to humans or animals (decision 2014/227/EU). - Product type-7, film preservatives (decision 2014/227/EU). - Product type-9, fibre, leather, rubber and polymerised materials preservatives (decision 2014/227/EU). |
| Switzerland | |
| Ordinance on Biocidal Products (OBP - SR 813.12) | Banned for - Product-type 1, human hygiene biocidal products (decision 2016/110/EU) - Product-type 2, disinfectants and algacides not intended for direct application to humans or animals (decision 2014/227/EU). - Product type-7, film preservatives (decision 2014/227/EU). - Product type-9, fibre, leather, rubber and polymerised materials preservatives (decision 2014/227/EU). |

No specific quality standard is set for triclosan under the Swiss Water Protection Ordinance.

Non-regulatory proposals for quality standards (QS), predicted no effect concentrations (PNEC) and environmental risk limits have been proposed by several national and international agencies within different contexts and following different derivation methods. Specifically for sediments, INERIS (2012) derived a QS_{sed} of 23 $\mu\text{g/kg d.w.}$ using the EqP. The Danish EPA (Miljøministeriet 2010) used the same approach but derived a QS_{sed} of 0.432 $\mu\text{g/kg d.w.}$, or 8.64 $\mu\text{g/kg d.w.} \times f_{OC}$ (fraction of organic carbon content in the sediment being assessed).

For general toxicity in surface waters, the Oekotoxzentrum (2017) proposed an AA-EQS of 0.10 $\mu\text{g/L d.w.}$ derived using a species sensitivity distribution (SSD) and an assessment factor (AF) of 5. This AA-EQS is also considered protective against secondary poisoning because the derived $QS_{sec.pois.}$ was 0.37 $\mu\text{g/L}$.

Additional values derived using approaches in line with the EU TGD have been derived. Schlich et al. (2014) derived an AA-EQS of 0.02 $\mu\text{g/L}$ from a 72 h test with *Pseudokirchneriella subcapitata* (0.2 $\mu\text{g/L}$) and AF of 10, also protective against secondary poisoning ($QS_{freshwater}$ for secondary poisoning derived at 0.48 $\mu\text{g/L}$). INERIS (2012) also derived a slightly lower $NQE_{EAU-DOUCE}$ than the AA-EQS from the Oekotoxzentrum, 0.05 $\mu\text{g/L}$, based on a NOEC for *Scenedesmus subspicatus* (0.5 $\mu\text{g/L}$) and AF of 10, while the Danish AA-EQS is set at 0.01 $\mu\text{g/L}$ (Miljøministeriet 2003).

An additional PNEC value, 0.058 $\mu\text{g/L}$, is provided by the Australian NICNAS (2009), value derived using a species sensitivity distribution (SSD) and AF of 5.



Table 3 Freshwater PNEC/quality standards available from authorities and reported in the literature.

| Description | Value | Development method | References |
|-------------------|--|--|---|
| <i>Sediment</i> | | | |
| QS_{sed} | 23 $\mu\text{g/kg d.w.}$ | EU TGD (EC 2011): Based on the EqP, derived for a sediment with 5 % OC and using a K_{oc} of 9200 L/kg ($\log K_{oc} = 3.96$) and a $QS_{freshwater}$ of 0.05 $\mu\text{g/L}$ | INERIS (2012) |
| QS_{sed} | 0.432 $\mu\text{g/kg d.w.}$ ($8.64 \times f_{oc}$) | EC TGD (2011): based on the EqP, derived for a sediment with 5 % OC and using a K_{oc} of 831.8 L/kg | Danish EPA, Miljøministeriet (2010) |
| <i>Water</i> | | | |
| AA-EQS | 0.10 $\mu\text{g/L}$ | EU TGD (EC 2011): derived from statistical extrapolation (SSD) and AF of 5. Protective against secondary poisoning ($QS_{freshwater}$ for secondary poisoning derived at 0.37 $\mu\text{g/L}$) | Oekotoxzentrum (2017) |
| $NQE_{EAU-DOUCE}$ | 0.05 $\mu\text{g/L}$ | EU TGD (EC 2011): Based on NOEC for <i>Scenedesmus subspicatus</i> (0.5 $\mu\text{g/L}$) and AF of 10. Protective against secondary poisoning ($QS_{freshwater}$ for secondary poisoning derived at 74 $\mu\text{g/L}$) | INERIS (2012) |
| AA-EQS | 0.02 $\mu\text{g/L}$ | EU TGD (EC 2011): derived from a 72-h test with <i>Pseudokirchneriella subcapitata</i> (0.2 $\mu\text{g/L}$) and AF of 10. Protective against secondary poisoning ($QS_{freshwater}$ for secondary poisoning derived at 0.48 $\mu\text{g/L}$) | Schlich et al. (2014) |
| $PNEC_{aquatic}$ | 0.058 $\mu\text{g/L}$ | ANZECC and ARMCANZ (2000) and EU TGD (EC 2011): derived from statistical extrapolation (SSD) and AF of 5 | NICNAS (2009) |
| $PNEC_{aquatic}$ | 0.01 $\mu\text{g/L}$ | EU TGD (EC 2003): Based on NOEC for <i>Scenedesmus subspicatus</i> (0.5 $\mu\text{g/L}$) and AF of 10 and additional AF of for endocrine effects | Danish EPA (Miljøministeriet 2010) |
| $PNEC_{aquatic}$ | 0.069 $\mu\text{g/L}$ | Based on NOEC for <i>S. subspicatus</i> (0.69 $\mu\text{g/L}$) and AF of 10 | Hanstveit and Hamwijk (2003) cited in NICNAS (2009) |

1.3 Use and emissions

Before its regulation, triclosan was included in many consumer products because of its broad antimicrobial activity against bacteria, as well as moulds and yeast. The main use of triclosan was in the formulation of cosmetic and personal care products such as toothpaste and deodorants, therapeutic products, veterinary products, pesticides, household cleaning products, textiles and grouting material, and as additive in plastic (SIDS OECD 2010; Oekotoxzentrum 2017).

Data on consumption in Switzerland and other countries are not available. According to Schlich et al. (2014), 40 tons per year were consumed in Germany as estimated for 1990, while Singer et al. (2002) reported a consumption of about 350 tons for Europe and of 450 tons in the USA, consistent with Dye et al. (2007) annual production and with the import volumes of triclosan in the order of 10 to 1000 tons for Europe (Windler et al. 2013 cited in Schlich et al. 2014).



These uses entail discharge to sewer and to natural surface waters after treatment. An additional source of triclosan to the aquatic environment is from applied biosolids, although this practice is not permitted in Switzerland.

Triclosan has been detected in waste water treatment plant effluents worldwide, including Switzerland (von der Ohe et al. 2011). Singer et al. (2002) studied triclosan occurrence and fate at the Gossau WWTP in Switzerland. The average dissolved concentrations of triclosan in the weekly flow-proportional composite samples ranged from 520 ng/L in the primary clarified effluent to 45 ng/L in the secondary effluent, which represented approx. 6 % of the total triclosan entering the plant. A mass flux analysis indicated that over one week study 79 % of triclosan was biologically degraded and 15 % was removed with the excess sludge, in addition to the 6 % leaving the plant in the effluent after the filtration stage. Concentrations in effluents from several WWTP ranged from 42 (Gossau) to 213 ng/L, corresponding to 0.2 to 3.2 g triclosan /day. Assuming that private households were the only sources of triclosan, the output load corresponded to 30-210 mg of triclosan/1000 inhabitants per day (study for 1999). Triclosan concentrations in the receiving water bodies were relatively constant, at approx. 20 ng/L, with concentrations increasing by a factor of 5 during high-water events, probably due to combined sewage overflow during rain events.

1.4 Mode of action

Triclosan is a biocidal product with multiple targets in the cytoplasm and membrane. At low concentrations, triclosan is a bacteriostatic agent¹ while at high concentrations it becomes a bactericidal (SCCS 2010). As a bacteriostat triclosan acts by blocking lipid synthesis through inhibition of the enzyme enoyl-acyl reductase (ENR) (McMurry et al. 1998 cited in Oekotoxzentrum 2017). Humans do not have an ENR enzyme and thus are not affected. However, studies with the plant *Arabidopsis* (family Brassicaceae) have shown that enoyl-acyl carrier protein reductase is a possible target of triclosan in plants (Serrano et al. 2007 cited in ECC & HC 2016). In mouse, the primary mode of action is activation of PPAR α which ultimately induces hepatocarcinogenesis (ECC & HC 2016). Triclosan is shown to alter thyroid hormone-associated gene expression in amphibians *in vitro* (Veldhoen et al. 2006 in ECC & HC 2016) and is suspected that triclosan can uncouple oxidative phosphorylation (ECC & HC 2016).

The presence of two phenol functional groups in triclosan suggests endocrine-disrupting potential of triclosan as already observed for other non-steroidal estrogens such as diethylstilbestrol and bisphenol A (Ishibashi et al. 2004 cited in Schlich et al. 2014). However, triclosan is not mentioned in the Community strategy for endocrine disrupters nor in the study report by DG ENV on updating the priority list of low tonnage chemicals (Petersen et al. al. 2007).

In the review performed for EQS derivation by Schlich et al. (2014), it is concluded that triclosan may interfere with the action of natural thyroid hormone in amphibians and freshwater organisms at concentrations of 1.5 $\mu\text{g/L}^2$. This concentration is 75-times higher than the lowest long-term NOEC of

¹ Bacteriostatic agents stop bacteria growth by inhibiting reproduction therefore upon removal of the bacteriostatic agent bacteria usually start growing again. Bactericide agents kill bacteria.

² According to Schlich et al. (2014): "Ishibashi et al. (2004) studied the effects of triclosan on the early life stages and reproduction of Japanese medaka (*Oryzias latipes*). Among other findings, they observed that gonadosomatic and hepatosomatic indices were significantly higher in adults exposed to concentrations of 20 $\mu\text{g/L}$ and higher. Also, concentrations of hepatic vitellogenin were increased significantly in males exposed to 20 and 100 $\mu\text{g/L}$ (Health & Environment Canada, 2012). Investigations by Foran et al. (2000) of possible estrogenic properties of triclosan on the same fish species indicated that this substance does not display estrogenic activity at levels ranging from 1 to 100 $\mu\text{g/L}$. In a study conducted on male western mosquitofish (*Gambusia affinis*), Raut and Angus (2010) observed a significant increase in normally female-limited vitellogenin mRNA expression at a



0.2 µg/L obtained in standard aquatic toxicity studies. It was concluded that the derived AA-QS_{freshwater} was protective regarding endocrine effects of triclosan on aquatic organisms.

Mihaich et al. (2017) performed a weight of evidence analysis addressing specific hypotheses related to interaction of triclosan with estrogen, androgen, and thyroid hormone pathways, and steroidogenesis using screening level studies in the US Endocrine Disruptor Screening Program and levels 1 through 5 of the OECD Conceptual Framework for Testing and Assessment of Endocrine Disruptors for multiple animals and in vitro studies, followed by a semiquantitative relevance weighting of each endpoint to a given hypothesis. These authors concluded that triclosan is not acting as an agonist or antagonist within the estrogen, androgen, thyroid, or steroidogenic pathways and is not impacting endocrine pathways as a primary mode of toxicity.

2 Environmental fate

2.1 Stability and degradation products

Triclosan will only slowly hydrolyse in contact with water, with half-lives estimated at > 1 year at 25°C and pH of 4, 7 and 9 (Ciba-Geigy 1990 cited in ECHA 2016). Significant photodegradation of triclosan in surface waters is much faster, with half-life < 1 h (Ciba-Geigy 1993 cited in ECHA 2016), direct phototransformation of the anionic form being the dominant photochemical degradation pathway (Tixier et al. 2002 cited in ECHA 2016).

Triclosan is not readily biodegradable according to 18-37 % triclosan degradation in 28 d OECD 301B and 0 % degradation in 28 d OECD 301C studies (Ciba-Geigy 1989, 1990 cited in ECHA 2016). However, the substance is inherently biodegradable in water according to OECD 302B studies, with >99 % elimination after 14 d of incubation (Ciba-Geigy 1999 cited in ECHA 2016), and several mineralization studies with activated sludge (ECHA 2016). Under anaerobic conditions less than 10 % degradation was observed (Colgate-Palmolive 1994 cited in ECHA 2016). Similarly, methyl-triclosan (CAS 4640-01-1), one of the metabolites of triclosan, is not readily biodegradable according to OECD 301B studies but is inherently biodegradable (ECHA 2016).

Biodegradation of triclosan was also studied in a water-sediment simulation study following OECD 308. The test was conducted under aerobic conditions with a mixed population from water and sediment as inoculum. Degradation of triclosan was monitored for 104 days using natural sediment from a pond and a river system. In both systems studied, triclosan dissipated very rapidly from the water to the sediments, with concentrations in the water phase representing on average 92.9 % (river) and 88.0 % (pond) immediately after application decreasing to 3.8 % and 6.5 % within 14 days of incubation. At the end of incubation, ¹⁴C-triclosan in the water phase reached mean amounts of 0.1 % and below detection limit. The concentration of ¹⁴C-triclosan in the total river and pond systems represented initially 92.9 % and 88.0 % and decreased to 21.4 % (river) and 21.8 % (pond) on day 104. Degradation of triclosan was observed in both compartments, but was more pronounced in the aqueous phases than in sediments. Mineralization assessed through CO₂ formation was 21.4 % (river) and 29.1 % (pond) of the applied radioactivity after 104 days of incubation. In sediment, the amount of non-extractable radioactivity steadily increased during incubation. At the end of incubation, means of 32.4 % and 33.0

triclosan treatment of 101 µg/L. In this study, which suggested that triclosan has the potential to act as an endocrine disruptor in male mosquitofish, it was also found that triclosan both decreased sperm counts and increased the mean hepatosomatic index at 101 µg/L. Triclosan has been shown to have endocrine disruption effects in amphibians at environmentally realistic concentrations. Studies do not demonstrate a consistent effect of triclosan on thyroid-mediated amphibian metamorphosis (Veldhoen et al., 2006). However, they demonstrated effects on developmental stage and a significant TRβ mRNA induction at 1.5 and 7.2 µg/L in a not dose-related manner (Fort et al., 2010 and 2011)".



% of the applied radioactivity remained unextracted from river and pond sediments, respectively. Further harsh extractions using acidic conditions under reflux extracted a maximum of 3.5 % of the applied radioactivity from the sediment on day 104. Subsequent organic matter fractionation of the non-extractable residues indicates that in both sediments the major part of the non-extractable radioactivity was bound to the immobile humin fraction amounting to mean amounts of 17.5 % and 20.2 % of the applied radioactivity for river and pond, respectively. Corresponding values for the fulvic acids were 7.5 % and 5.0 % and for the humic acids 4.0 % and 6.0 %. Half-lives, calculated using first order kinetics, were 1.2 d for water, 56.4 d for sediment and 41.1 for the total river system; and 1.4 d for water, 56 d for sediment and 58.3 d for total pond system (ECHA 2016). This study reported sixteen minor metabolites, including methyl-triclosan (highest amounts of 4.8 % on day 104 in river system, sediment extract) and M8 (highest amount of 6.5 % at day 56 in river) in the water phases or sediments of both systems. At the end of the study (day 104) their amounts were ≤ 5.5 %.

Biodegradation in soil was studied in a simulation study with three different soils following OECD Guideline 307 (Aerobic and Anaerobic Transformation in Soil). Triclosan dissipation half-lives were 2.46-2.68 d at 20°C and 10.7 d at 10°C. Triclosan was primarily transformed to methyl-triclosan (no information on % in ECHA 2016), which had half-lives at 20°C from 39 to 153 days depending on the soil type (ECHA 2016).

NICNAS (2009) presents a comprehensive review of biodegradation and methylation of triclosan by sewage sludge microorganisms under aerobic and anaerobic conditions. According to several OECD and non-standard test studies, biodegradation of triclosan by wastewater microorganisms is very slow under anaerobic conditions relative to aerobic conditions. The rate of biodegradation is inversely proportional to the triclosan exposure concentration, with inhibition occurring at higher exposure concentrations. However, microbial community adaptation to triclosan has been demonstrated and lengthening the duration of exposure enables relatively greater removal of triclosan by biodegradation even at relatively higher exposure concentrations (see NICNAS 2009 for primary studies). Methyl-triclosan also forms during aerobic treatment of sewage and is discharged in sewage effluent together with residues of triclosan. This metabolite occurs at much lower concentrations than triclosan (Bester 2003 in NICNAS 2009 estimation is 1 % conversion rate of triclosan to methyl-triclosan during secondary treatment), although methylation of triclosan may also continue post-treatment in the receiving environment (NICNAS 2009).

2.2 Sorption/desorption processes

Triclosan has shown to deposit rapidly in sediments in dissipation studies (see section 2.1). Sediment water partitioning coefficients (K_d) from batch equilibrium studies with freshwater sediments range from 203 to 1572 L/kg, with geomean value of 837 L/kg (Table 1). Average suspended matter water partitioning coefficient from estuarine field studies reported by Wilson et al. (2009) is 9000 L/kg. Soil water partitioning coefficients from batch equilibrium studies range from 1.3 to 273.2 L/kg, below those reported in batch equilibrium studies with freshwater sediments. These additional values reported for suspended matter from estuarine areas and soils are considered less relevant in the context of this report and are not used for EQS derivation.

Normalized organic carbon water partition coefficients ($\log K_{oc}$) for triclosan derived experimentally from sediment batch studies range from 3.90 to 5.26. These values are higher than those reported at ECHA (2016) obtained using OECD 121 method of 2.62 and 2.92 but are in good agreement with pseudo-partitioning coefficients experimentally derived from field studies in freshwater environments. Wang and Kelly (2017) reported an average $\log K_{oc}$ of 4.54 from a thirteen month survey in the tropical urban catchment in Singapore, consisting of a highly urbanized area and tributaries flowing through industrial and residential intensive areas. Zhang et al. (2013) also reported an average $\log K_{oc}$ of 4.8 from an extensive field study in the Dongjiang River.



The information available on the influence of organic carbon (OC) on triclosan partitioning in sediments from laboratory and field studies is scarce. Zhang et al. (2013) showed an apparent increasing binding at increasing OC and clay content in sediments from Dongjiang River (Zhang et al. 2013). In laboratory batch experiments, Huang et al. (2015) found a higher adsorption capacity (K_d) in sediments with higher OC suggesting the adsorption of triclosan is primarily attributed to the hydrophobic interaction with organic materials in sediments. In this study, the adsorption capacity of sediments decreased as the concentration of triclosan increased, and a higher percentage of triclosan desorbed at increasing concentrations, likely due to the saturation of the adsorption sites in sediments.

According to triclosan pKa of 8.01-8.14, sorption of triclosan seems to be highly sensitive to pH in sediments. According to ECC & HC (2016), the Multispecies Model (version 1.0; Cahill 2008 in ECC & HC 2016) estimates that when triclosan is exclusively released to water, it is expected to reside in both water (79–91 %) and sediment (9–21 %) at pH 7 and 8, respectively. If released only to soil, triclosan remains almost exclusively in this compartment (>99 %). At an environmental pH of 7, triclosan will mainly be present in its neutral form in water, sediment and soil. At a pH of 8 in these same compartments, about 55% of triclosan will be in its neutral form and about 45 % in its ionized (anionic) form. The estimated partitioning coefficients were derived from studies at pH < 8. According to estimation cited in Lyndall et al. (2010), such experiments are expected to underestimate K_{OC} , because they do not account for slow adsorption phenomena or for sorption irreversibility, whereby desorption K_{OC} can greatly exceed adsorption K_{OC} . This explains the higher K_{OC} values reported in triclosan partitioning from in situ sediments (Wilson et al. 2009). Lyndall et al. (2010) also cite that modelling effects of pH and OC on K_{OC} of triclosan indicate that effects of pH are minor compared with the variation in K_{OC} associated with differences among sediment OC types (Seth et al. 1999 in Lyndall et al. 2010).

2.3 Bioavailability

Bioavailability is a complex process which depends on many factors including the sorption capacity of the sediment considered (e.g. OC content), the hydrophobicity of the compound, and the physiology, feeding behaviour and burrowing activity of the benthic organism considered (Warren et al. 2003). For ionisable substances such as triclosan, pH can also play a role in bioavailability.

No study specifically dealing with triclosan bioavailability in sediments could be located. Lyndall et al. (2010) performed a probabilistic risk assessment for triclosan in water and sediments and concluded that increased pH would result in increased bioavailability of triclosan in sediment but lower toxicity, although it was argued that these countervailing effects may cancel one another under more alkaline conditions. However, no quantitative relationship between pH and toxicity was available.

Rowett et al. (2016) studied the toxicity of triclosan in the amphipod *Gammarus pulex* in water exposures and evaluated the effects of two different environmental pH of 7.3 and 8.4, which affect triclosan dissociation, different dissolved organic carbon (humic acid) concentrations (11 and 16 mg/L) and different exposure durations (24 and 48 h). EC₅₀ at 48h exposures at pH 8.4 were almost 50 % higher than the mean EC₅₀ at pH 7.3. Addition of humic acids also increased EC values compared with tests with alike pH conditions. Therefore toxicity tests at pH above triclosan pKa and in the presence of humic acids result in significantly decreased triclosan toxicity, attributed by the authors to most likely varying triclosan speciation and complexation due to triclosan's pKa and high hydrophobicity controlling its bioavailability. When tests were performed with waste water treatment plant effluent, the resulting EC values were higher than those obtained at similar levels of OC as added humic acid, suggesting that the type of OC also has an effect on triclosan toxicity. The mechanisms controlling this decreased bioavailability could not be elucidated due to interaction among the evaluated factors.



It is not known how other exposure routes (sediment ingestion, food quantity and quality) contribute to triclosan bioavailability and therefore toxicity.

2.4 Bioaccumulation and biomagnification

Several bioaccumulation studies are cited in NICNAS (2009), ECHA (2016) and Arnot et al. (2018) for triclosan with different fish species, concentrations and duration (Table 4). Due to time constraints the reliability assessment as performed by Arnot et al. (2018) following Arnot and Gobas (2006) has been taken forward and studies have not been assessed further for this report.

The only studies assessed as acceptable by Arnot et al. (2018) were the OECD 305 studies performed as part for the Japan's Chemical Substance Control Law reporting bioconcentration factors (BCF) for common carp of 23 and 53 L/kg w.w. for 3 and 30 µg/L (CERI 1992, NITE 2012 cited in Arnot et al. 2018). The lower BCFs are attributed to being based on parent chemical only (rather than total radioactivity). Additional BCF are present for two other studies, assessed with low reliability. BCF calculated for zebrafish in flow-through studies (5 weeks duration) following OECD guideline 305C were 4157 L/kg w.w. at a concentrations of 3 µg/L and 2532 L/kg w.w. at 30 µg/L. After 2 weeks of depuration, loss reached 98 - 99 % (Ciba-Geigy Ltd. 1991 cited in ECHA 2016). Schettgen et al. (1999 cited in ECHA 2016 and Arnot et al. 2018) also derived BCF (25 d exposure) of 7900 L/kg w.w. at pH 6 and 35.9 µg/L initial concentration and 3740 L/kg w.w. at a pH of 9 and 46.7 µg/L.

Table 4 Bioaccumulation factors (BCF) from laboratory studies with adult fish.

| Method/guideline | Species | Exposure duration | BCF/BAF/BSAF | Reliability ^a | Reference |
|------------------|--|-------------------|--|--|--|
| OECD 305 | Common carp (<i>Cyprinus carpio</i>) | 56 d | 23 L/kg w.w. (3 µg/l) 53 L/kg w.w. (30 µg/l) | Acceptable (none identified, some information not available) | CERI (1992) and NITE (2012) in Arnot et al. (2018) |
| OECD 305 C | Zebrafish (<i>Danio rerio</i>) | 5 weeks | 4157 L/kg w.w. (3 µg/l) 2532 L/kg w.w. (30 µg/l) | Low (total radiolabel; nonspecific chemical analysis) | Ciba-Geigy Ltd. (1991) in ECHA (2016) and Arnot et al. (2018) |
| OECD 305 D | Zebrafish (<i>Danio rerio</i>) | 25 d | 7900 L/kg w.w. (35.9 µg/l, pH 6) 3740 L/kg w.w. (46.7 µg/l, pH 9) | Low (nonspecific chemical analysis) | Schettgen et al. (1999) in ECHA (2016) and Arnot et al. (2018) |

^a As assessed by Arnot et al. (2018) according to Arnot and Gobas (2006). In parenthesis key sources of uncertainty.

Several field monitoring studies confirm the presence of triclosan in aquatic organisms in Germany, Japan, Sweden, Switzerland, the Netherlands and the United States, with concentrations in the low ng/g range and increasing concentrations in native and caged organisms close to waste water treatment plant effluents (NICNAS 2009). Rüdél et al. (2013) reported concentrations of triclosan in archived fish samples from German rivers (16 sites, including the Elbe and Rhine) for the period 1994-2003 and 2008 in the range <0.2–3.4 ng/g w.w. (muscle), corresponding to <2–69 ng/g lipid weight, without apparent concentration trends over time.



Field studies show that the transformation product methyl-triclosan is bioaccumulated to a larger extent than the parent compound, in agreement with slightly higher log K_{OW} (NICNAS 2009; log K_{OW} of 5.2 in Lyndall et al. 2010). Rüdell et al. (2013) report methyl-triclosan concentrations in archive fish samples from German rivers one order of magnitude higher than those of triclosan (see paragraph above), in the range 1.0–33 ng/g w.w. (muscle), corresponding to 47–1010 ng/g lipid weight. In a field study performed in Swiss lakes in 2000 and 2002, methyl-triclosan was detected in all fish samples in the range <2 to 365 ng/g corresponding to about <0.01 to 35 ng/g w.w. except in fish from remote lakes (Balmer et al. 2004). Estimated bioaccumulation factors (BAF) for methyl-triclosan from measured concentrations in fish and water concentrations quantified using semi-permeable membrane devices were 2000–5200 L/kg w.w. assuming an average fat content in the fish of 2 % (Balmer et al. 2004).

Estimated BAF for different invertebrates are reported in the review by Arnot et al. (2018), ranging from 900 to 2100 L/kg w.w. for algae, 500 for snails, 340 L/kg w.w. for mussels, 102–112 L/kg w.w. for clams and 130 L/kg w.w. for marine mussels. Similar BAFs were estimated using the AQUAWEB food web model for phytoplankton, zooplankton, deposit-feeding and filter-feeding invertebrates. The resulting BAFs from the AQUAWEB model for small, medium and large fish were 175, 140 and 113 L/kg w.w., adding evidence according to Arnot et al. (2018) to the conclusion that the BCF for triclosan is < 2000 L/kg. The Biomagnification Factors (BMF) reported by Arnot et al. (2018) from the AQUAWEB model are 0.22 kg/kg (zooplankton), 0.35 kg/kg (small fish), 0.55 kg/kg (medium fish) and 0.65 kg/kg (large fish).

Concerning the risk of benthic invertebrates to transfer toxic and bioaccumulative substances to higher trophic levels, the EFSA scientific opinion for sediment risk assessment proposes to perform spiked sediment bioaccumulation tests with benthic invertebrates for substances that show significant bioaccumulation in fish (BCF ≥ 2000) when the substance is (1) persistent in sediment (DT₅₀ >120 d in water-sediment fate studies) and log K_{OW} >3; or (2) non-persistent in sediment, log K_{OW} >3 and >10 % of the substance found in the sediment in a water-sediment fate study (EFSA 2015). There are several laboratory studies that have reported bioaccumulation of triclosan in oligochaetes. Peng et al. (2018a) exposed the oligochaete *Limnodrilus hoffmeisteri* to triclosan in microcosms during 28 days, reporting BSAF ranging between 0.38–3.55 for triclosan concentrations of 0.8, 8 and 80 µg/g d.w. A bioaccumulation model accounting for accumulation through water and sediment (ingestion) compartments was used to describe bioaccumulation over time, indicating that the system reached steady state at the end of the experiment and that virtually all bioaccumulated triclosan was taken up from sediment across all tested concentrations. In a 14 days bioaccumulation study, Peng et al. (2018b) reported BSAF of 2.07 at 3 µg/g d.w. triclosan exposure. Dang et al. (2016) also reported BSAF for the oligochaete *Lumbriculus variegatus* after 28 d of exposure of 1.4 when exposed to triclosan at sediment concentration of 1.4 µg/g d.w. in a sediment with a very high OC content (39 %). Karlsson et al. (2016) reported a much higher BSAF of 9.04 for *L. variegatus* exposed for 48 h to sediment concentration of 186 µg/g d.w. (nominal) and <1 % OC. An additional BSAF was estimated at 6.61 µg/g d.w. for non-feeding *L. variegatus* obtained by removing anterior segments with a razor blade in this last study, which can be attributed to accumulation solely through the dermis from the dissolved phase. Differences in the BSAF are probably related to different sediment characteristics (e.g. OC) and test design, but also it is highlighted that these BSAFs are maximum values as they were based on radioactivity representing both parent and transformation products but results were not analytically confirmed.

3 Analysis

3.1 Methods for analysis and quantification limit

Triclosan is quantified in sediment extracts reaching limits of detection or quantification as low as 10 µg/kg d.w. by high performance liquid chromatography-tandem mass spectrometry (HPLC-MS/MS)



with electrospray ionization (Peng et al. 2018b) and gas chromatography–mass spectrometry (Pintado-Herrera et al. (2014).

Table 5 Methods for triclosan analysis in sediments and corresponding limits of detection (LOD) and limits of quantification (LOQ) ($\mu\text{g}/\text{kg}$ d.w.).

| LOD | LOQ | Analytical method | Reference |
|------|------|-------------------|-------------------------------|
| -- | 0.10 | LC–ESI–MS/MS | Peng et al. (2018b) |
| 0.10 | -- | GC–MS | Pintado-Herrera et al. (2014) |

3.2 Environmental concentrations

Measured environmental concentrations (MEC) of triclosan in sediments are summarized in Table 6. The concentration of triclosan in surface sediments from Lake Lugano was $20 \mu\text{g}/\text{kg}$ d.w. (Chiaia et al. 2014), while concentrations in surface sediments from Lake Greifensee were $53 \mu\text{g}/\text{kg}$ d.w. in 1998 (Singer et al. 2002) and $40 \mu\text{g}/\text{kg}$ d.w. in 2010 (Chiaia et al. 2014). Singer et al. (2002) reported maximum concentrations of triclosan in Lake Greifensee in the deeper layers corresponding to sediments dated to the mid-1970s of $75 \mu\text{g}/\text{kg}$ d.w., showing the high persistence of triclosan in the lake. Similar concentrations have been reported in other areas of the world, with maximum concentrations reported in China (Zhao et al. 2013). Higher concentrations of triclosan are usually found in sewage impacted streams (tributaries) and lower concentrations are usually located in larger rivers.

Table 6 Measured environmental concentrations (MEC) of triclosan in Switzerland and other areas of the world. All concentrations expressed as $\mu\text{g}/\text{kg}$ d.w. for sediment if not indicated otherwise.

| Country | MEC (min-max) ^a | No. of sites | Comments | Reference |
|-------------|--|--------------|---|-------------------------------|
| Switzerland | 53 | 1 | Lake Greifensee, surface sediment, 1998 | Singer et al. (2002) |
| | 40 | 1 | Lake Greifensee, surface sediment | Chiaia et al. per.comm |
| | 20 | 1 | Lake Lugano, surface sediment | Chiaia et al. (2014) |
| Spain | (0.3-9.6) | 13 | Estuary of Guadalete River | Pintado-Herrera et al. (2014) |
| China | Main river: (<1.58-196) Tributaries: (<1.58-1329) | | Chinese rivers, surface sediments, 2007-2009 | Zhao et al. (2013) |
| US | 19.5 (2-26) 21.2 (14-34) | 6 | Hudson river estuary, surface sediment, 2006 and 2007 | Wilson et al. (2009) |
| US | (<0.6-110) | 10 | Santa Clara River watershed, Surface sediment | Maruya et al. (2016) |

^a When measured at more than 1 site, average values are reported.

4 Effect data (spiked sediment toxicity tests)

A non-filtered bibliographic search was performed for Triclosan in the US EPA Ecotoxicity Data Base (U.S. EPA 2020) which did not yield data on sediment organisms. A key word search was performed on Web of Science and PubMed (Triclosan AND sediment OR benthic OR benthos), no restriction regarding publication date which resulted in 265 publications, with duplicates removed. Of the 265 publications, 13 were identified as potentially relevant based on an initial screen of abstracts. An additional search



was also performed on Web of Science and PubMed (Triclosan AND mesocosm OR microcosm), no restriction regarding publication date which resulted in 56 publications, with duplicates removed. None of these 56 publications were identified as potentially relevant based on an initial screen of abstracts.

Relevance (“C” score in Table 7) and reliability (“R” score in Table 7) of studies are evaluated according to the CRED-criteria (Moermond et al. 2016) adapted for sediments (Casado-Martinez et al. 2017).

According to the EU TGD (EC 2018) “What is considered chronic or acute is very much dependent on 1) the species considered and 2) the studied endpoint and reported criterion”. According to EFSA, true chronic tests should cover a range of 28-65 d when half-life of a pesticide in sediment is >10 d (EFSA 2015). Therefore, effect data from 10 d tests with *Ampelisca abdita* and *Mysidopsis bahia* (Perron et al. 2012) were considered as acute effect data.

The chronic effect data for the marine sea urchin *Lytechinus variegatus* and the mussel *Perna perna* (Pusceddu et al. 2018) were considered not directly useful for EQS derivation because not enough information was available for assessing reliability and relevance. They are retained as supportive information.

Peng et al. (2018a) produced effect concentrations from a microcosm study, the effect datum for *Limnodrilus hoffmeisteri* is considered reliable with restrictions and can be directly used in EQS derivation. The effect datum for the snail *Bellamya* sp. was considered not reliable due to the small number of individuals tested and is used as supportive information.

Two studies reported effect data for biological communities. The microcosm study which assessed effects of triclosan in microbial communities is assessed as not relevant because functional endpoints were not provided. They are retained as supportive information. The microcosm study is also assessed as not reliable and will be used as supportive information because only two concentrations were tested and due to not conclusive information on the OC content.

Supportive information will be used for example in choosing the assessment factor (AF).



Table 7 Reliable and relevant sediment effect data collection for triclosan in mg/kg d.w. Data were evaluated for relevance and reliability according to the CRED criteria for sediments (Casado-Martinez et al. 2017). Data used for QS development is underlined. Abbreviations: n. a. = not available.

| Group | Species | Test compound | Exposure | Equilibration time | Endpoint | Test duration | Effect concentration | Value [mg/kg d.w.] | Sediment type | Normalized value [mg/kg d.w., 1% OC] | Normalized value [mg/kg d.w., 5% OC] | Chem. analysis | Note | Validity | References |
|-------------------------------------|--|---------------|----------|---|----------------------------------|---------------|----------------------|--------------------|---|--------------------------------------|--------------------------------------|----------------|---|----------|----------------------|
| Acute toxicity data in freshwater | | | | | | | | | | | | | | | |
| No data available | | | | | | | | | | | | | | | |
| Acute toxicity data in marine water | | | | | | | | | | | | | | | |
| Amphipoda | <i>Ampelisca abdita</i> | Triclosan | Static | At least one week | Survival | 10 d | LC50 | 260 | Natural sediment, 2 % organic carbon (OC), salinity 30 % | 130 | 650 | Measured | Chemical analysis performed, sampling time not reported, both organisms exposed in same beakers | R4/C3 | Perron et al. (2012) |
| Mysidacea | <i>Mysidopsis bahia</i> | Triclosan | Static | | Survival | 10 d | LC50 | 256 | | 128 | 640 | Measured | | R4/C3 | |
| Chronic toxicity data in freshwater | | | | | | | | | | | | | | | |
| Oligochaeta | <i>Limnodrilus hoffmeisteri</i> (in multi-species test, including 5 algal species, <i>Daphnia magna</i> and 4 th instar midge larvae) | Triclosan | Static | 3 d (plus 4 d pre-equilibration by mixing manually the spiked sediment for 5 min) | Survival | 28 d | NOEC | 7.415 | Natural sediment, clay (56%), silt (43%), and sand (0.65%), 1.9% organic matter (OM), 0.04% total phosphorus, 0.16% total nitrogen, and 0.01% ammonia nitrogen (NH ₃) | 6.74 | 33.7 | Measured | NOEC derived from time-average measured concentration. OC = OM/1.72 = 1.1%, microcosm study | R2/C1 | Peng et al. (2018a) |
| Mollusca | <i>Bellamya sp.</i> | Triclosan | | | Survival | 28 d | NOEC | 7.415 | | 6.74 | 33.7 | Measured | NOEC derived from time-weighted measured concentration. OC = OM/1.72 = 1.1%, microcosm study Not reliable due to low number of individuals per replicate | R3/C1 | |
| Bacterial community | <i>Different species</i> | Triclosan | Static | 4 d plus 3 d in test system | Richness, evenness and structure | 28 d | NOEC | 8 | Natural sediment, clay (56%), silt (43%), and sand (0.65%), 1.9% organic matter (OM), 0.04% total phosphorus, 0.16% total | 7.27 | 36.4 | Measured | NOEC derived from measured concentration on Day 28. | R2/C3 | Peng et al. (2019) |



| Group | Species | Test compound | Exposure | Equilibration time | Endpoint | Test duration | Effect concentration | Value [mg/kg d.w.] | Sediment type | Normalized value [mg/kg d.w., 1% OC] | Normalized value [mg/kg d.w., 5% OC] | Chem. analysis | Note | Validity | References |
|---------------------------------------|---|---------------|--------------|--------------------|--|---------------|----------------------|--------------------|--|--------------------------------------|--------------------------------------|----------------|--|----------|------------------------|
| | | | | | | | | | nitrogen, and 0.01% ammonia nitrogen (NH ₃) | | | | OC = OM/1.72 = 1.1%. Not relevant, absence of functional endpoints | | |
| Chronic toxicity data in marine water | | | | | | | | | | | | | | | |
| Sea urchin | <i>Lytechinus variegatus</i> | Triclosan | Static | 7 d | Embryo-larval development | 24 h | NOEC | 0.0075 | Natural sediment, 7.6% of coarse sand, 27.7% of medium sand, 56.8% of fine sand, 0.7% of very fine sand, 7.2% of silt and clay, 22.1% of carbonates and 0.36% of OM. Salinity 35 ‰ | 0.0357 | 0.178 | Measured | Chemical analysis performed, sampling time not reported OC = 0.36/1.71=0.21 | R4/C2 | Pusceddu et al. (2018) |
| Mollusca | <i>Perna perna</i> | Triclosan | Static | 7 d | Embryo-larval development | 48 h | NOEC | 0.0075 | Natural sediment, 7.6% of coarse sand, 27.7% of medium sand, 56.8% of fine sand, 0.7% of very fine sand, 7.2% of silt and clay, 22.1% of carbonates and 0.36% of OM. Salinity 35 ‰ | 0.0357 | 0.178 | Measured | Chemical analysis performed, sampling time not reported OC = 0.36/1.71=0.21 | R4/C2 | Pusceddu et al. (2018) |
| Mesocosm data | | | | | | | | | | | | | | | |
| Microcosm ^a | Marine meio- and macrobenthic communities | Triclosan | Flow-through | - | Total abundance, taxonomic richness, and diversity | 14 d | NOEC | 13.9 | Uncontaminated field core, authors used 2% OC for normalization | 6.95 | 34.8 | Measured | NOEC derived from measured concentration on Day 3 OC/OM not reported | R3/C2 | Ho et al. (2013) |

^a Different sediment layers of tested sediment core included the field sediment, a treatment sediment with spiked triclosan, and a DNA-free sediment layer.



4.1 Graphic representation of effect data

As there is only one reliable and relevant study in the sediment dataset for triclosan no graphical representation of the data has been generated.

4.2 Comparison between marine and freshwater species

Statistical comparison of marine and freshwater effect data is not possible due to the very limited amount of available data.

4.3 Overview of reliable and relevant long-term studies

According to the EC EQS TGD (EC (2018) p. 25): “All available data for any taxonomic group or species should be considered, provided the data meet quality requirements for relevance and reliability”.

The chronic effect data for *Limnodrilus hoffmeisteri* (survival) has been evaluated as reliable with restrictions based on available information in published papers by Peng et al. (2018a). In the following, information on the critical study on *Limnodrilus hoffmeisteri* (survival) is summarized.

Peng et al. (2018a) “Fate and effects of sediment-associated triclosan in subtropical freshwater microcosms”.

- Species: *Limnodrilus hoffmeisteri*
- No standardised guideline was followed, and the study was not conducted according to the principles of GLP.
- Study set-up: microcosms with a range of test organisms (40 midges, 240 worms, 6 snails, 30 daphnids, and algae at a density of approximately 104 cells/mL per microcosm).
- Origin of test organisms: juvenile worms were purchased from an aquatic market (Guangzhou, South China) and placed into separate 18-L glass holding tanks with aerated tap water and unbleached tissue paper as substrate. Worms with similar size and mass (representing similar age) were selected and cultured for 2 weeks in the laboratory at the same light and temperature conditions as the microcosm experiment
- Experimental sediment: sediment was collected in September 2015 from an uncontaminated site (Liuxi Reservoir, Guangzhou, South China). The sediment was wet sieved through a 300 µm sieve using deionized water to remove potential benthic macroinvertebrates. The sieved sediment contained 62 % water. The sediment was composed primarily of clay (56 %), silt (43 %), and sand (0.65 %). It contained 1.9 % organic matter (OM), 0.04 % total phosphorus, 0.16 % total nitrogen, and 0.01 % ammonia nitrogen (NH₃).
- Spiking and equilibration time: sediment was spiked with triclosan dissolved in acetone. After spiking, the sediment was thoroughly mixed for 30 min in a stainless steel mixer. Further mixing was performed manually for 5 min using a spade during the following four days. Before introduction to the microcosms, each spiked sediment was further mixed for 20 min using the stainless steel mixer. The same volume of acetone (6.45 mL) was added to all concentrations. Both solvent control and water control were included by replacing triclosan stock solution with the same volume of acetone and aerated Milli-Q water, respectively.
- Overlying water: aerated tap water (12.6 L; 0.056 % total organic carbon (TOC), 0.001 % total phosphorus, 0.164 % nitrate (NO₃⁻), 0.0002 % nitrite (NO₂⁻) and 0.030 % (NH₃).
- Bioassays: indoor glass microcosms (30×30×20 cm) in a temperature-controlled room (27 ± 1 °C). After introduction of spiked sediment and aerated tap water, the particles in the water column were allowed to settle for 3 days before addition of the test organisms. Test exposure comprised 8 microcosms plus one sacrificed at start for chemical measurements in the overlying water and sediment (day 0). 4 replicates had sediment and water only (i.e., without test organisms) and 4 with sediment, water, and test organisms. Microcosms were illuminated



with a cool white fluorescent light (2200 lx) and a daily photoperiod of 12 h. Each microcosm was aerated using a glass pipette connected to an aeration system. During the experiment, evaporated water was replenished with aerated tap water weekly to maintain the original water level. Nitrogen (0.7 mg/L as urea) and phosphorus (0.09 mg/L as triple super phosphate) were added biweekly to the systems to provide nutrients for algal growth. The relatively high concentration of NH_3 and further addition of nutrients adds uncertainty to the reliability of the study.

- Test duration: 28 days.
- Tested concentrations: 0.8, 8, 80, 240 $\mu\text{g/g}$ d.w. (nominal). Spacing between the three lowest concentrations is 10. This spacing is relatively high and above recommendations for spiked-sediment toxicity testing for NOEC derivation.
- Test endpoints: Survival after 28 d
- Measured concentrations: concentrations in the overlying water and sediment were determined at the start (day 0) and end (day 28) of the experiment. Concentration in water samples was extracted using solid-phase extraction (SPE), while in sediment samples were extracted by ultrasonic extraction combined with SPE purification. Extracts were analysed by high performance liquid chromatography-tandem mass spectrometry (HPLC-MS/MS) with electrospray ionization (ESI) in the negative mode. By the end of experiment concentrations in the sediment decreased by 3.43 ± 0.56 – 11.76 ± 0.64 % in systems with introduced organisms.
- Statistics: no observed effect concentrations (NOECs) were calculated using the Williams test which assumes a concentration-effect relationship. The Williams tests were performed using the Community Analysis computer program, version 4.3.05. In order to down-weight high abundance values and obtain approximately a normal distribution of the data, the abundance values of species were $\ln(Ax+1)$ transformed, where x represents the abundance data and A was set as 2 to avoid false discrepancy between zero abundance values and low abundance values.
- Results: survival NOEC = 7.41 mg/kg d.w. (time-averaged measured concentration); 8 mg/kg d.w. (nominal concentration).

5 Derivation of QS_{sed}

According to the EC TGD for EQS, sediment toxicity tests, aquatic toxicity tests in conjunction with equilibrium partitioning (EqP) and field/mesocosm studies are used as several lines of evidence to derive QS_{sed} (EC 2018). Thus, in the following, the appropriateness of the deterministic approach (AF-Method), the probabilistic approach (SSD method) and the EqP approach were examined.

5.1 Derivation of $QS_{sed, AF}$ using the Assessment Factor (AF) method

The derivation of $QS_{sed, AF}$ is determined using assessment factors (AFs) applied to the lowest credible datum from long-term toxicity tests.

The lowest long-term effect datum available for triclosan is the NOEC of 7.415 mg/kg d.w (Table 8) for the survival of *Limnodrilus hoffmeisteri*.

Table 8 Most sensitive relevant and reliable chronic data summarized from Table 7.

| Species | Exposure duration [d] | Endpoint | NOEC/ EC_{10} [mg/kg d.w.] | OC [%] |
|---------------------------------|-----------------------|----------|------------------------------|--------|
| <i>Limnodrilus hoffmeisteri</i> | 28 d | Survival | 7.415 | 1.1 |



In case of long term tests (NOEC or EC₁₀) being available for a single benthic species, the TGD recommends the application of an assessment factor of 100 (Table 11 in EC (2018)).

The application of an AF of 100 to the lowest credible chronic datum results in a QS_{sed,AF} = 74.1 µg/kg d.w., which corresponds to 337 µg/kg d.w. for a sediment with 5 % OC or 67.4 µg/kg d.w. for a sediment with 1 % OC representing a worst case scenario in Switzerland.

5.2 Derivation of QS_{sed,SSD} using the species sensitivity distribution (SSD) method

The minimum data requirements recommended for the application of the SSD approach for EQS water derivation is preferably more than 15, but at least 10 NOECs/EC₁₀s, from different species covering at least eight taxonomic groups (EC (2018), p. 43). In this case, not enough data from spiked sediment toxicity tests are available for applying the SSD approach.

6 Derivation of QS_{sed,EqP} using the Equilibrium Partitioning approach

If no reliable sediment toxicity data are available, the Equilibrium Partitioning (EqP) can be used to estimate the EQS_{sed,EqP}. This approach, developed for non-ionic substances (Di Toro et al. 1991), is used here for comparison purposes given the small data base of sediment toxicity studies.

6.1 Selection of QS for water

Several environmental risk limits and quality standards are available for triclosan in water (section 1.2). For the derivation of the EQS_{sed,EqP}, a PNEC for the aquatic freshwater environment derived with a methodology similar to the procedure described in the TGD for deriving the AA-EQS for freshwater (e.g. with regard to the AF) should be used.

The QS_{FW-ECO} used for the calculation of the QS_{sed,EqP} based on direct toxicity using the equilibrium partitioning approach is 100 ng/L (0.1 µg/L) derived by the Oekotoxzentrum (2017). This QS_{FW-ECO} allows harmonization at the national level and is also protective for top predators from secondary poisoning.

6.2 Selection of partition coefficient

One of the main factors influencing the application of the EqP model is the choice of the partition coefficient. It is stipulated in the ECHA 2017 guideline (p. 143, ECHA (2017)) that “To increase the reliability of PNEC sediment screen derived using the EqP, it is imperative that a conservative but realistic partitioning coefficient (e.g. K_d, K_{OC}, K_{OW}) is chosen. A clear justification must be given for the chosen coefficient and any uncertainty should be described in a transparent way.”

The EC EQS TGD requires deriving a geometric mean of all available K_{OC} values including one derived from a log K_{OW} value (EC 2018).

Estimates of the organic carbon normalised partition coefficient (K_{OC}) are available from six studies with sediments, and also by calculation from K_{OW}. The average (geometric mean) K_{OC} value is 36353 (log K_{OC} 4.56) (Appendix I). The K_{sed-water} value calculated from this K_{OC} value is 183 for 1 % TOC.

6.3 Selection of OC content for a reference sediment

To account for the influence of OC content on QS_{sed,EqP} development, calculations have been performed for a standard sediment according to the EU TGD with 5 % OC (EC 2018). As 5 % OC might not be representative for sediment in Switzerland, calculation was made as well for a worst case scenario considering measurement on total sediment with 1 % OC (approx. 10th percentile of OC content in Swiss Rivers).



6.4 Derivation of QS_{sed,EqP}

The QS_{FW-ECO} used for the calculation of the QS_{sed,EqP} based on direct toxicity using the equilibrium partitioning approach is 100 ng/L (0.1 µg/L).

The QS_{sed,EqP} for triclosan based on K_{OC} data is 70.0 µg/kg w.w. for a sediment with 5% OC, or a value of 14.1 µg/kg w.w. for a sediment with 1% OC.

The QS_{sed,EqP} for triclosan based on K_{OC} data is 182 µg/kg d.w. for a sediment with 5 % OC, or a value of 36.6 µg/kg d.w. for a sediment with 1 % OC.

As triclosan has a log K_{OW} value lower than 5 an additional assessment factor of 10 is not warranted.

Table 9 Derived QS_{sed,EqP} for a mean K_{OC} based on Appendix I and the EQS derived from Oekotoxzentrum (2017). The partition coefficient solid-water sediment (K_{p,SED}) is estimated for a sediment with 5 % OC (standard EC TGD sediment) and 1 % TOC (worst case scenario in Switzerland).

| | K _{OC} [L/kg] | K _{p,SED} [L/kg] | K _{sed-water} [m ³ /m ³] | PNEC _{water} [µg/L] | QS _{sed,EqP} [µg/kg w.w.] | QS _{sed,EqP} [µg/kg d.w.] | Included AF |
|--------|---------------------------|------------------------------|---|---------------------------------|---------------------------------------|---------------------------------------|----------------|
| 1 % OC | 36353 | 364.5 | 183 | 0.1 | 14.04 | 36.5 | -- |
| 5 % OC | 36353 | 1821 | 910 | 0.1 | 70.0 | 181.9 | -- |

7 Determination of QS_{sed} according to mesocosm/field data

No relevant and reliable mesocosm/field data is available for triclosan. Although the microcosm study from Ho et al. (2013) was reported as mesocosm study it was performed using sediment cores exposed in the laboratory so they cannot be classified as mesocosm for EQS derivation.

8 Toxicity of transformation products

According to available data, methyl-triclosan is one of the main transformation products of triclosan in soil, sediment and sewage. This metabolite occurs at much lower concentrations than triclosan. Singer et al. (2002) estimated that approx. 5 % of triclosan concentration is present as methyl-triclosan in sediments from Lake Greifensee. Pintado-Herrera et al. (2014) reported concentrations of methyl-triclosan ranging from <0.1 to 1.8 µg/kg d.w. in estuarine sediments, with average 0.925 µg/kg d.w. and detection frequency of 60 % (n=1) while triclosan concentrations at the same sites ranged from 0.3 to 9.6 µg/kg d.w. and 100 % detection frequency although the proportion of methyl-triclosan compared to the triclosan concentrations were much higher than 5 % as estimated by Singer et al. (2002). Similar range of methyl-triclosan concentrations were quantified in archived suspended matter from German rivers by Rüdell et al. (2013). Methyl-triclosan is however more persistent and apparently more bioaccumulative.

Detailed information on its ecotoxicity to benthic invertebrates was not available for review. However, there are effect concentrations of methyl-triclosan in laboratory studies for several aquatic organisms. Methyl-triclosan and triclosan showed similar toxicity to zebrafish *Danio rerio*, with a NOEC of 160 µg/L (nominal concentration) in 144 h post hatching lethal and sub-lethal endpoints for both the parent and transformation product (Macedo et al. 2017). The sea urchin (*Paracentrotus lividus*) also showed higher toxicity when exposed to methyl-triclosan than to triclosan, with LOEC of 1 µg/L for methyl-triclosan and 160 µg/L for triclosan for larval length at 48 h post hatching development tests (Macedo et al. 2017). On the contrary, a 72 h bioassay with algae *Scenedesmus subspicatus* reported an EC50 on growth rate at 170 µg/L for methyl-triclosan (Bätscher 2006 cited in Macedo et al. 2017) while a geomean of 1.94 µg/L is reported in the triclosan EQS derivation dossier from the Oekotoxzentrum



(2017). Similarly, Villa et al. (2014) reported IC₅₀ values for *Allivibrio fischeri* (formerly known as *Vibrio fischeri*, Microtox test system) of 1.76 mg/L for methyl-triclosan and 0.73 mg/L for triclosan. For *Daphnia magna*, the 48 h immobilization assay reported a NOEC of 180 µg/L for methyl-triclosan (Bätscher 2006 cited in Macedo et al. 2017) while the EC₅₀ for immobilization for *D. magna* is reported as 258 µg/L (geomean, Oekotoxzentrum 2017). Overall, these results indicate that the toxicity of the transformation product methyl-triclosan should not be neglected as it can be more toxic than the parent compound for some aquatic organisms.

9 EQS_{sed} proposed to protect benthic species

The different QS values for each derivation method included in the EC EQS TGD 2018 are summarized in Table 10. According to the TGD, the most reliable extrapolation method for each substance should be used (EC 2018). In all cases, data from spiked sediment toxicity tests are preferred over the EqP approach.

Table 9 QS_{sed} derived according to the three methodologies stipulated in the EU-TGD and their corresponding AF. All concentrations expressed as µg/kg d.w.

| | Sediment 1 % TOC | Sediment 5 % TOC | AF |
|-----------------------------------|---------------------|---------------------|-----|
| QS _{sed,SSD} | - | - | - |
| QS _{sed,EqP} | 36.5 | 182 | - |
| QS _{sed,AF} | 67.4 | 337 | 100 |
| Proposed EQS_{sed} | 67.4 | 337 | |

An EQS_{sed} of 67.4 µg/kg (1 % OC) for triclosan is proposed for protecting benthic organisms. For protection against secondary poisoning, the QS_{sed,EqP} could be used.

9.1 Uncertainty analysis

The EQS_{sed} is set at the 67.4 µg/kg d.w. This EQS_{sed} is derived to protect benthic invertebrates and is derived from a NOEC for the oligochaete *L. hoffmeisteri*, which has several limitations (see section 4 and 4.3 specifically). However, this study is supported by the effect data for freshwater mussels and microbial community structure, and a microcosm study (marine). Additional 10 d effect data for the marine amphipod *A. abdita* and the mysid *M. bahia* are available. It is noted that the study used for EQS_{sed} derivation has several limitations.

The data base used in the derivation of the AA-EQS for surface waters (Oekotoxzentrum 2017) taken further for QS_{sed,EqP} derivation also includes effect data for several sediment-relevant organisms, including the freshwater amphipod *Hyaella azteca* (LC₁₀ of 5 µg/L) and the midge *Chironomus tentans* (LC₁₀ of 20 µg/L). The use of the EqP to convert these effect concentrations in sediment concentrations results in values in the same order of magnitude as the effect data available from long-term spiked sediment toxicity testing in Table 7 (1826 and 7303 µg/kg d.w. for 1 % OC, respectively). This is in agreement with the acute effect data reported in the Oekotoxzentrum (2017) database, with a 96 h EC₅₀ for mortality of 2840 µg/L for *Chironomus plumosus* and 2046 µg/L for *L. hoffmeisteri*, which indicate similar toxicity for these two organisms in water-only exposures. These concentrations are much higher than those reported in surface waters from the microcosm study that derived the NOEC used in QS_{sed,AF} derivation, attributed by the authors to pH differences, 8.0 in the water-only exposure and 7.5 in the water-sediment microcosm study taking into account that triclosan in neutral form is



more toxic than in ionic form (Orvos et al. 2002), and the presence of sediment and therefore the addition of uptake from pore water and sediment may contribute also to higher toxicity in sediment-relevant organisms as *L. hoffmeisteri*.

According to the database in water-only exposures, the most sensitive taxa are microalgae and cyanobacteria, for which no effect data based on spiked-sediment toxicity tests is available. However, these are covered by the $QS_{sed,EqP}$, which is within a factor 2 of the proposed EQS_{sed} based on the $QS_{sed,AF}$.

Uncertainties remaining in triclosan EQS derivation include some uncertainty in the endocrine potential of triclosan and the development of antimicrobial resistance. This endpoint is being assessed at present within the new prioritisation phase for the EU WFD initiatives and may be addressed when the triclosan EQS is updated.

The transformation product methyl-triclosan is also accumulated in sediment and may be more toxic to some aquatic organisms than the parent compound.

The proposed EQS_{sed} is considered preliminary according to the high AF used in its derivation according to the relatively low number of effect data from long-term spiked-sediment toxicity tests available.

No analytical issues are foreseen for the implementation of the derived EQS_{sed} .



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Appendix I. Sediment-water partition coefficient (K_{oc}) coefficient

| TOC, type | | Log K_{oc} | K_{oc} | Reference/Source |
|---|------|--------------|--------------|--|
| OECD guideline 121, HPLC method | exp. | 2.92 | 831 | ECHA (2016) |
| OECD guideline 121, HPLC method | exp. | 2.62 | 417 | ECHA (2016) |
| Sewage sludge, 45.4 % OC | exp. | 4.68 | 47 454 | ECHA (2016) |
| Field study, freshwater sediment (n=16), OC 1.23-7.17 pH 7.63 \pm 0.54; 4.54 \pm 1.40 | exp. | 4.54 | 34674 | Wang and Kelly (2017) |
| Field study, freshwater sediment (n=94), OC 0.1-10.6; 4.80 \pm 0.53 | exp. | 4.8 | 63096 | Zhao et al. (2013) |
| Batch simulation study, freshwater sediment, OM 2.44 % Clay 26.4 % pH 6.8 | exp. | 4.95 | 88951 | Calculated from Lin et al. (2011) |
| Batch simulation study, freshwater sediment, OM 2.97 % Clay 19.5 % pH 6.8 | exp. | 4.90 | 79600 | Calculated from Lin et al. (2011) |
| Batch simulation study, freshwater sediment, OM 1.05 % Clay 13.3 % pH 6.8 | exp. | 5.40 | 253548 | Calculated from Lin et al. (2011) |
| OECD 106 Batch equilibrium study, freshwater sediment, OC 1.0 % Clay 65.7 % pH 8.4 | exp. | 4.17 | 14712 | Recalculated from Huang et al. (2014) |
| OECD 106 Batch equilibrium study, freshwater sediment, OC 3.53 % Clay 45.1 % pH 5.9 | exp. | 4.61 | 40374 | Recalculated from Huang et al. (2014) |
| OECD 106 Batch equilibrium study, freshwater sediment, OC 4.09 % Clay 60.5 % pH 7.9 | exp. | 4.22 | 16769 | Recalculated from Huang et al. (2014); Wu et al. (2015) |
| Batch equilibrium study, freshwater sediment, OC 1.37 pH 7.7 Clay 7.0 % | exp. | 4.17 | 14803 | Styszko (2016) |
| Batch equilibrium study, freshwater sediment, OC 1.83 pH 7.6 Clay 8.5 % | exp. | 4.46 | 29022 | Styszko (2016) |
| Batch equilibrium study, freshwater sediment, OC 2.03 pH 7.6 Clay 18.2 % | exp. | 5.26 | 181330 | Styszko (2016) |
| OECD 106 Batch equilibrium study, freshwater sediment, OC 0.5 % Clay 0.9 % | exp. | 3.90 | 8000 | dos Santos et al. (2018) |
| Estimated from K_{ow} (4.90) | est. | 3.90 | 7943 | Log K_{oc} = 0.63*log K_{ow} + 0.90 Log K_{oc} = 0.57*log K_{ow} + 1.08 |
| | | 4.56 | 36353 | Geomean |
| Simulation study OPPTS 835, biosolid (n=16), OC 27.6-45.9 % pH 6.08-11.8; 4.30 \pm 0.44 | exp. | 4.3 | 19953 | Agying-Birikorang et al. (2010) |
| Simulation study OPPTS 835, soil (n=4), OC 0.03-0.31 pH; 4.24 \pm 0.52 | exp. | 4.24 | 17378 | Agying-Birikorang et al. (2010) |



| | | | | |
|---|------|------|-------|--|
| Simulation study OPPTS 835, biosolid-amended soil (n=16); 4.26±0.35 | exp. | 4.26 | 18197 | Agying-Birikorang et al. (2010) |
| Batch simulation study, soil, OC 0.44 pH 7.51 Clay 3.6 % | exp. | 3.34 | 2188 | Xu et al. (2009) |
| Batch simulation study, soil, OC 0.55 pH 7.06 Clay 12.5 % | exp. | 4.38 | 23988 | Xu et al. (2009) |
| Batch simulation study, soil, OC 1.03 pH 7.48 Clay 42.5 % | exp. | 3.94 | 8710 | Xu et al. (2009) |
| Batch simulation study, soil, OC 3.16 pH 7.14 Clay 18.1 % | exp. | 3.56 | 3631 | Xu et al. (2009) |
| Clay soil, pH 7.4, OC 1.9 % | exp. | 3.29 | 1958 | Waller and Kookana (2009); Kookana et al. (2011) |
| Sandy soil, pH 5.4, OC 0.9 % | exp. | 2.97 | 939 | Waller and Kookana (2009); Kookana et al. (2011) |
| Batch simulation study, soil, OC 0.1-5.4 pH 5.8-10.4 Clay 1.2-26; range 3.12-3.92 N=4 | exp. | 3.56 | 3631 | Roberts et al. (2014) |
| Batch simulation study, soil, sand OC 0.1 Clay 0 % | exp. | 3.99 | 9772 | Karnjanapiboonwong et al. (2010) |
| Batch simulation study, soil, sandy loam OC 1.3 pH 8.3 Clay 16 % | exp. | 4.30 | 19953 | Karnjanapiboonwong et al. (2010) |
| Batch simulation study, soil, silty loam OC 1.5 pH 7 Clay 12 % | exp. | 4.05 | 11220 | Karnjanapiboonwong et al. (2010) |