Biodegradation During Sand Filtration – EFSA-ECHA Water Treatment Guidance Document.

Introduction

Supporting information, delete before finalization: Assessment required for each substance that is found in raw water at concentration ≥0.1 µg/L at the point of abstraction for drinking water production.

The joint guidance of EFSA (European Food Safety Authority) and ECHA (European Chemicals Agency),[1] provides detailed information about the impact of water treatment processes on active substances (AS) and their environmental transformation products (eTP) when abstracted for drinking water production, and the resulting treatment transformation product (tTP) formation. The assessment of the formation of tTPs is thereby a stepwise process. This begins with an assessment of the relevant environmental concentrations of both AS and its eTPs in groundwater and surface water using associated FOCUS modelling to derive predicted environmental concentrations (PEC's) in drinking water (PEC_{dwa}) of AS or eTP. If it is considered that a compound is potentially present in groundwater or surface water ≥ 0.1 µg/L, for an AS or eTP of a plant protection product (PPP) at the point of abstraction of raw water, experimental studies are triggered including chlorination, ozonation, and UV disinfection. Furthermore, the guidance features sand filtration as the key component covering biodegradation in natural environments and filter beds during sand and activated carbon filtration within specific hydraulic retention times.

The following OECD study types are considered to address environmental biodegradation:

- OECD 307: Aerobic and anaerobic transformation in soil
- OECD 308: Aerobic and anaerobic transformation in aquatic sediment systems
- OECD 309: Aerobic mineralization in surface water
- OECD 314: Simulation tests to assess the biodegradability of chemicals discharged in wastewater

The EFSA/ECHA water treatment guidance emphasizes the difficulties in comparing sand filters used in water treatment practices and OECD environmental biodegradation study designs. Differences in filter contact time, microbial communities and characteristics of the sand in the filters may affect biodegradation kinetics and the formation of tTPs when comparing real conditions in drinking water facilities with the suggested OECD study types. Although there are stark study differences, the guidance document clearly emphasizes that the "*microbially mediated transformation products in rapid sand filters will be comparable to those already identified in OECD 307, 308 and 309 studies*". As an alternative, activated sludge from municipal wastewater treatment plants is suggested as a worst-case model to identify potential microbial transformation products when above-mentioned OECD tests are unavailable.

If tTPs are identified in the individual experimental laboratory studies at concentration of ≥0.075 µg/L, a subsequent hazard risk assessment must be conducted. As there is a concentration threshold approach for tTPs, concentrations of tTPs must be derived from the proposed sand filtration/biodegradation

[1] ECHA and EFSA (European Chemicals Agency and European Food Safety Authority); Hofman-Caris, R.; Dingemans, M.; Reus, A.; Shaikh, S. M.; Muñoz Sierra, J.; Karges, U.; aus der Beek, T.; Nogueiro, E.; Lythgo, C.; Parra Morte, J. M.; Bastaki, M.; Serafimova, R.; Friel, A.; Court Marques, D.; Uphoff, A.; Bielska, L.; Putzu, C.;… Papadaki, P. (**2023**). Guidance document on the impact of water treatment processes on residues of active substances or their metabolites in water abstracted for the production of drinking water. EFSA Journal, *21*(8), 1–108. https://doi.org/10.2903/j.efsa.2023.8194

studies in the water treatment guidance document. To address this requirement, the concentrations of potential tTPs resulting from a typical biodegradation process (OECD 307, 308, 309, 314) cannot directly be retrieved from the experimental data as the original experiments were not designed to describe this unique water treatment process. Thus, an alternative approach must be derived which considers the water treatment process in question, the degradation of the input substance and its predicted environmental concentration in raw water at drinking water abstraction points.

There are assumptions that can be made to define these necessary parameters when assessing conventional rapid sand filtration and resulting tTP formation.

1) Rapid sand filtration processes are not more biologically active than soil
   Rapid sand filtration is essentially a physical process, relying on mechanical filtration to remove suspended particles and other turbidity. Rapid sand filtration is used when high-throughput water treatment is required and to avoid need for large areas of land to achieve the required rate of treatment of high volumes of water. Hence, they are commonly used in municipal drinking water facilities.[2-3] Thus, given the way that biological activity develops in sand filtration beds, the rapid sand filtration system can be considered significantly less biologically active than soil environments.

2) The time available for potential substance biotransformation is defined by the water residence time.
   Given operational high rates of water throughput for rapid sand filters, typical residence times are of the order of 10 minutes,[4] but residence times of no more than 60 minutes are used in rapid gravity biofilters.[5] Although no consolidated EU-wide statistics are publicly available, estimates can be derived from technical literature, and the WISE database.[6] See **Table 1** for further details.

   Table 1: Estimated residence times for filtration practices used across Europe during drinking water treatment practices.

Technique	Estimated Share in Europe	Typical Residence Time	Typical Use Case	Key Features
Rapid Gravity Biofilter (RBGF)	~50-60%	15-30 minutes	Large municipal treatment plants	High flow rate, biological activity in filter bed
Rapid Sand Filtration	Included in RGBF share	5-15 minutes	Municipal and industrial systems	Physical filtration, limited biological activity
Pressure Sand Filters	~10-20%	5-15 minutes	Industry, decentralized systems	Compact, pressurized, mini

Impact Assessment

According to the joint guidance of EFSA and ECHA[1], XXX is considered to be potentially present in groundwater or surface water at a concentration ≥0.1 µg/L, at the point of abstraction of raw water (the PEC_{dwa} for XXX was X.XX µg/L).

[2] Drinking Water Quality Regulator for Scotland (DWQR); https://dwqr.scot/media/jl0ddz3x/pws-technical-manual-section-6-water-treatment-processes-65-filtration-larger-scale.pdf
[3] United States Environmental Protection Agency (EPA) (**1990**). Technologies for Upgrading Existing or Designing New Drinking Water Treatment Facilities; https://nepis.epa.gov/Exe/ZyPURL.cgi?Dockey=300048WU.txt
[4] Hedegaard, M. J.; Albrechtsen, H.-J. *Water Res.* **2014**, *48*, 71-81.
[5] Moona, N.; Holmes, A.; Wünsch, U. J.; Pettersson, T. J. R.; Murphy, K. J. *ACS ES&T Water* **2021**, *1*, 1117-1126.
[6] European Environment Agency (EEA), WISE Water Framework Directive Database.

Therefore, the concentration of tTPs formed during representative sand filtration during water treatment processes was assessed using the available data from studies conducted according to *delete as appropriate:* OECD 307, OECD 308, OECD 309 and OECD 314 guidelines.

All available rate of degradation OECD study data for XXX was assessed to investigate whether a single treatment transformation product could potentially be formed as a result of sand filtration processes, at a concentration of ≥0.075 µg/L, using **Equation 1**.

Equation 1:

$$[tTP]_{max} = [C]_0 \left(1 - \exp\left(\frac{-\ln 2}{DT_{50}} \times t\right)\right)$$

Where:

- $[tTP]_{max}$ = predicted concentration of a single transformation product in treated water (units of µg/L).
- $[C]_0$ = concentration of substance being evaluated (AS or eTP) in raw water, equivalent to PEC_{dwa} (units of µg/L). This is equivalent to the selected concentration for lab simulations (e.g. ozonation, chlorination, UV treatment).

Supporting information for section below, delete before finalization: Proposal that choice of DT50 to be left up to individual applicants (modelling SFOs / geomeans etc.)

- DT_{50} = first-order biodegradation half-life (*e.g.*, in soil, total system water/sediment, aerobic mineralisation) (units of $days^{-1}$). This is equivalent to the $DT_{50,modelling}$ of the substance being evaluated (AS or eTP) from OECD 307 (OECD 308 or OECD 309, respectively) studies.
- t = water residence time in the rapid sand filtration apparatus (units of days). Rapid sand filtration occurs with a residence time of <60 minutes (equivalent to 0.04167 days).

Supporting information for section below, delete before finalization: AS or eTP DT50s from cold studies or acquired from parent studies are appropriate for Tier 1 assessment Propose to have one table per study type (OECD 307/308/309)

For XXX, available rate of degradation OECD study data was evaluated, and $[tTP]_{max}$ were calculated for each compartment and associated kinetic parameters using **Equation 1**. The results are detailed below in **Table 1**:

Table 1: The predicted maximum concentration of a single tTP during a representative sand filtration during water treatment processes for XXX, calculated using available OECD 307/308/309 study data.

Study Reference	Compartment (Soil/Sediment/Water)	$[C]_0$ (µg/L)	$DT_{50,modelling}$ (days)[a]	$[tTP]_{max}$ (µg/L) using Equation 1
Study 1	Soil 1		XXX	XXX
Study 1	Soil 2		XXX	XXX
Study 1	Soil 3		XXX	XXX
Study 2	Soil 1		XXX	XXX
Study 2	Soil 2		XXX	XXX
Study 2	Soil 3		XXX	XXX

a) Modelling endpoints derived using SFO kinetics.

Either

The calculations and results outlined in **Table 1** indicate that tTPs would not be generated at ≥0.075 µg/L as a result of sand filtration during water treatment processes. Accordingly, no further investigation of degradation products formed during sand filtration is required.

Supporting information, delete before finalization: Or if any $[tTP]_{max}$ ≥0.075 µg/L, then follow on higher tier assessment required this is only necessary for specific soils or environmental compartments where the calculations in Table 1 indicate the potential to produce tTPs at a concentration ≥0.075 µg/L

A higher tier approach was considered where tTPs would potentially be generated at ≥0.075 µg/L as a result of sand filtration during water treatment processes. The studies in consideration are detailed in **Table 2**.

Supporting information for section below, delete before finalization: In table, only include those soils/compartments that have triggered further assessment.

Table 2: Studies for further consideration where $[tTP]_{max}$ ≥0.075 µg/L as a result of sand filtration during water treatment processes.

Study Type (OECD 307/308/309)	Study Reference	Compartment (Soil/Sediment/Water)	DT_{50}, modelling (days)[a],	$[tTP]_{max}$ (µg/L) using Equation 1
OECD 307	Study 1	Soil 1	XXX	XXX
OECD 308	Study 2	Sediment 1	XXX	XXX
OECD 309	Study 3	Natural Water 1	XXX	XXX

a) Modelling endpoints derived using SFO kinetics.

Supporting information for section below, delete before finalization: 14C data where an AS or eTP is dosed to the test system should be used for the Tier 2 assessment. If no 14C data is available and the Tier1 assessment is >0.075 µg/L then you would need to consider generating additional data to address this e.g. OECD314.

Available route data from the corresponding OECD studies can be used to calculate the expected concentration of each tTP, based on the concentration of the substance being evaluated (AS or eTP in raw water), ($[C]_0$) and the occurrence of the tTP formed at timepoint relevant for sand filtration (% AR, as percentage of applied radioactivity from the corresponding OECD study). Using this available OECD data, the concentration of the tTP during a representative sand filtration during water treatment processes can be calculated using **Equation 2** based on the occurrence of the tTP at the first available timepoint after 0 DAT, and a correction of the molecular weight of the tTP.

Equation 2:

$$[tTP]_{max} = [C]_0 \left(1 - \exp\left(\frac{-\ln 2}{DT_{50}} \times t\right)\right) \times \text{Max. Occ.}_{tTP} \times \frac{\text{Mw}_{tTP}}{\text{Mw}_{\text{AS or eTP}}}$$

Where:

- $[tTP]_{max}$ = concentration of a single transformation product in treated water (units of µg/L).
- $[C]_0$ = concentration of substance being evaluated (AS or eTP) in raw water, equivalent to PEC_{dwa} (units of µg/L). This is equivalent to the selected concentration for lab simulations (e.g. ozonation).

- DT_{50} = first-order biodegradation half-life (*e.g.*, in soil, total system water/sediment, aerobic mineralisation) (units of $days^{-1}$). This is equivalent to the $DT_{50,modelling}$ of the substance being evaluated (AS or eTP) from OECD 307 (or OECD 308 or OECD 309, respectively) studies.
- t = water residence time in the rapid sand filtration apparatus (units of days). Rapid sand filtration occurs with a residence time of <60 minutes (equivalent to 0.04167 days).
- $Occ._{tTP}$ = maximum occurrence of the tTP at first available timepoint after 0 DAT from the OECD 307, 308 and 309 studies (units of %). This is equivalent to % AR in the OECD studies.
- Mw_{tTP} = Molecular weight for the tTP (units of g/mol).
- $Mw_{AS\ or\ eTP}$ = Molecular weight for the substance being evaluated (AS or eTP) (units of g/mol).

The tTP concentrations, using available OECD study data, were calculated using **Equation 2** and the occurrence of each eTP at the first available timepoint after 0 DAT. The tTP concentrations are presented in **Table 3** (full OECD study data is presented in **Appendix XXX**, which was copied from the AS DAR (AS DAR, YEAR), and the degradation scheme for the transformation of XXX is presented in **Appendix XXX**).

Table 3: The predicted concentration of tTPs during a representative sand filtration during water treatment processes for XXX, calculated using data from OECD study data (XXX applied).

Supporting information for section below, delete before finalization: This only applies to the substance being dosed to the test system.

Substance under evaluation = XXX; **PEC_{dwa} = $[C_0]$ (µg/L)** = XXX

Compound	**Molecular Weight, Mw (g/mol)**	**First Avaialble Timepoint**	**Mean max occurrence (%)**	**[tTP] (µg/L) using Equation 2**
Soil / Compartment – Study Reference *Supporting information for section below, delete before finalization: Overview of study which max single tTP > 0.075 can be possible. Take first avaialble timepoint after 0 DAT and give metabolites formed, MW, % AR and resulting predicted concentration. Metabolites in question are only those that have been identified in the corresponding OECD studies.*				
eTP 1 (i.e. metabolite from XXX applied OECD study under investigation)	XXX	XX DAT	XXX	XXX
eTP 2 (i.e. metabolite from XXX applied OECD study under investigation)	XXX		XXX	XXX
Soil / Compartment – Study Reference				
eTP 1 (i.e. metabolite from XXX applied OECD study under investigation)	XXX	XX DAT	XXX	XXX
eTP 2 (i.e. metabolite from XXX applied OECD study under investigation)	XXX		XXX	XXX

Either

This approach demonstrates that there could be a tTP generated at a concentration ≥0.075 µg/L as a result of sand filtration during water treatment processes on XXX, predicted from a combination of OECD study data, PEC_{dwa} and a conservative filter bed residence time (using the first available timepoint from OECD study data). The maximum predicted concentrations of the generated tTPs are reported in **Table 4**.

Table 4: Maximum predicted concentration of tTPs during a representative sand filtration during water treatment processes for XXX, calculated using data from OECD study data (XXX applied).

Sand Filtration tTP	Maximum Predicted Concentration (µg/L)
XXX	XXX
XXX	XXX
XXX	XXX

This is considered a conservative approach as rapid sand filtration processes are unlikely to be more biologically active than soil, and the time available for substance biotransformation is defined by the water residence time (~60 minutes), which is significantly shorter than the first available timepoint from the selected OECD study data. Treatment transformation products and their calculated concentrations as outlined in Table 4 should then be used as input parameters for the consumer risk assessment of these transformation products

OR

This approach demonstrates that there will not be a tTP generated at a concentration ≥0.075 µg/L as a result of sand filtration during water treatment processes on XXX, predicted from a combination of OECD study data, PEC_{dwa} and a conservative filter bed residence time (using the first available timepoint from OECD study data).

OR

DT_{50} data derived from non-radiolabelled studies or determined via formation of metabolites from an upstream precursor (parent) are appropriate for the assessment of whether total degradation ≥0.075 µg/L as calculated using **Equation 1** and summarised in **Table 1.** Only data derived from [^{14}C]-labelled OECD studies where the substance being investigated was dosed as the test item to the test system can be used to assess the route of transformation and the formation amounts of any transformation products formed (**Equation 2, Table 3**). As no [^{14}C]-data is available for XXX, and the Tier 1 assessment results in a $[tTP]_{max}$ = ≥0.075 µg/L, an OECD 314 study should be conducted to assess whether any relevant transformation products are formed at a concentration ≥0.075 µg/L.

Conclusion

According to the joint guidance of EFSA and ECHA[1], XXX was identified as an (AS or eTPs) that could be present in groundwater or surface water above 0.1 µg/L at the point of abstraction of raw water. Therefore, the concentration of tTPs during a representative sand filtration during water treatment processes was assessed using the available data from studies conducted according to OECD 307, 308 and 309 guidelines for these compounds. The OECD 307, 308 and 309 experiments were not designed to describe this unique water treatment process and the use of them is considered conservative, because rapid sand filtration processes are unlikely to be more biologically active than soil and the time available for substance biotransformation is defined by the water residence time, which will be significantly shorter than the study duration.

In an initial assessment, using the rate of degradation from OECD study data, the maximum concentration of a single tTP, formed during a representative sand filtration during water treatment processes was calculated based on an appropriate residence time for rapid filtration processes, in combination with the compartmental DT_{50} value in OECD 307, 308 and 309 studies for XXX and the maximum PEC_{dwa}.

Insert conclusions as appropriate

Further refinement of the assessment was undertaken where tTPs were shown to be ≥0.075 µg/L, using a residence time of 60 minutes to calculate the expected concentration of tTPs as a result of biodegradation during sand filtration. Using the OECD study data, the concentration of the tTP undergoing a representative sand filtration during water treatment processes was calculated based on the occurrence of the tTP at the first available timepoint after 0 DAT and a correction of the molecular weight of the tTP. This is considered conservative because typically rapid sand filtration occurs with a residence time of <60 minutes.

Using a refined approach, there will not be a tTP generated at a concentration ≥0.075 µg/L as a result of sand filtration during water treatment processes on XXX, predicted from a combination of OECD study data, PEC_{dwa} and a conservative filter bed residence time (using the first available timepoint from OECD study data).

APPENDIX XX: Proposed degradation pathway for XXX

APPENDIX XX: Rate of degradation in OECD studies

APPENDIX XX: Route of degradation in OECD studies