



ECHO-News

Chlorothalonil-metabolites

Chlorothalonil is an active ingredient that was used in plant protection products as a fungicide against fungal infestations in agriculture. At the beginning of 2020 the authorization by the European Union was not extended. By the use of the active ingredient Chlorthalonil degradation products (metabolites) could arise and reach the groundwater¹.

For this reason the LANUV NRW carried out a non-target screening to obtain informations on the occurrence of **chlorothalonil metabolites** in ground- and surface water.

Chlorothalonil metabolite R417888

Molar mass: 329,54 g/mol Molecular formula: C₈H₃Cl₃N₂O₄S

 $\begin{array}{l} log \; D_{pH \; 7} : - \; 0,7 \\ K_{fOC} : \; 4,6\text{-}17 \; mL/g \\ DT_{50} : \; 62\text{-}1000 \; d \end{array}$

H₂N CI OH

Chlorothalonil metabolite R471811

Molar mass: 347,56 g/mol Molecular formula: C₈H₅Cl₃N₂O₅S

 $\begin{array}{l} log \ D_{pH \ 7} : -1,7 \\ K_{fOC} : not \ available \\ DT_{50} : 98\text{-}1000 \ d \end{array}$

Analytiks

The analytical determination of six chlorothalonil metabolites was carried out by LC-MS/MS after direct injection (DIN 38407-36), allowing the quantification from mass concentrations above 0.025 µg/L.

To confirm the positive findings of chlorothalonil metabolite R417888 and chlorothalonil metabolite R471811 a second independent LC-MS/MS method after sample clean-up and chromatography on a HILIC separation column was used.

Occurrence

Two of six chlorothalonil metabolites tested (R471811 and R417888) were detected in the ground- and surface water samples, and the established health guidance value (GOW) of 3 μ g/L was not exceeded in any sample. Most findings were detected in groundwater. For the metabolite R471811, the maximum value in groundwater was 0.74 μ g/L. In surface water, the concentrations were in the range of 0.05 μ g/L - 0.29 μ g/L. The following figures show the individual matrices and monitoring sites.

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¹https://www.eawag.ch/fileadmin/Domain1/Beratung/Beratung_Wissenstransfer/Publ_Praxis/Faktenblaetter/fb_chlorothalonilmetaboliten_d.pdf

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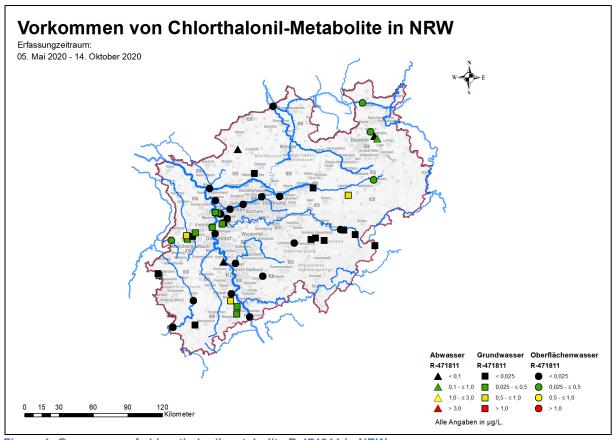


Figure 1: Occurrence of chlorothalonil metabolite R-471811 in NRW

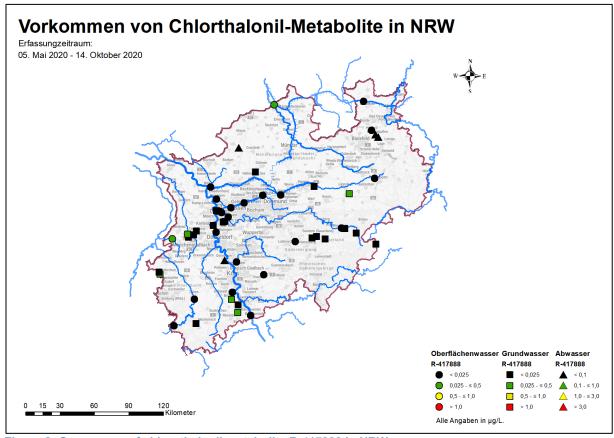


Figure 2: Occurrence of chlorothalonil metabolite R-417888 in NRW

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Table 1: Studied Chlorothalonil metabolites

Name	Sum formula	Substance group
Chlorothalonil metabolite R417888	$C_8H_3CI_3N_2O_4S$	Sulphonic acid
Chlorothalonil metabolite R471811	$C_8H_5CI_3N_2O_5S$	Sulphonic acid
Chlorothalonil metabolite R611968	$C_8H_3CI_3N_2O_2$	Phenol
Chlorothalonil metabolite SYN507900	$C_8H_3CI_3N_2O_2$	Phenol
Chlorothalonil metabolite SYN548580	$C_8H_5CI_3N_2O_3$	Phenol
Chlorothalonil metabolite SYN548581	$C_8H_3CI_3N_2O_4S$	Sulphonic acid

Relevance

According to the "GOW list" of the UBA $(2019)^2$, the chlorothalonil metabolites R471811 and R417888 are so-called "non-relevant metabolites" for which a health guidance value (GOW) of 3 μ g/L has been set.

According to the findings, the metabolite R471811 is particularly conspicuous; it is readily soluble in water and considered to be difficult to remove. For the removal of the substance in drinking water treatment, only reverse osmosis is a suitable process. Other processes such as activated carbon, UV disinfection or ozonisation are only suitable to a limited extent or are unsuitable³. Based on the data available so far, this metabolite is potentially relevant to drinking water.

No ecotoxicological data are available for the substance. Due to the low log P, no high bioaccumulation potential is expected. Available data indicate that the substance is persistent in the environment.

Further procedure

Two valid methods are available at the LANUV for the determination of chlorothalonil metabolites in water bodies. According to the available data, no additional findings to those already obtained are expected from further regular measurements. In case of special questions, specific investigations can be performed.

Impressum

Herausgeber

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²https://www.umweltbundesamt.de/sites/default/files/medien/374/dokumente/gowpflanzenschutzmetabolite 0.pdf

³European Food Safety Authority (**2018**) Conclusion on the peer review of the pesticide risk assessment of the active substance chlorothalonil. *EFSA Journal*. 16(1):5126, 47 pp. doi:10.2903/j.efsa.2018.5126 - Appendix A

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What are ECHO News?

Current events consistently bring compounds or groups of substances into discussion for which no pollution information is available for the aquatic environment in North Rhine-Westphalia and beyond.

The **ECHO** program was established in order to be able to make short-term relevance statements, e.g. on the impact on the drinking water supply. **ECHO** pursues the goal of evaluating new substances with possible water relevance "on demand".

ECHO News provides a first relevance statement for this individual compound/substance group immediately after measurement results are available.

In case of water relevance based on this assessment, detailed results and systematic evaluation are published in **ECHO** substance reports.

ECHO documents are available at https://www.lanuv.nrw.de/umwelt/umweltanalytik/echo-schnelle-relevanzpruefung-fuer-neue-stoffe.