

US EPA ARCHIVE DOCUMENT

Summary of Data Submissions in Support of the Me Too Registration

Aqueous Photolysis 161-2 (MRID 45710223)

The aqueous phototransformation of [¹⁴C]tetrachloroisophthalonitrile (chlorothalonil), at a nominal concentration of 0.3 mg a.i./L, was studied at 25 ± 1°C in sterile aqueous pH 7 (0.01M phosphate) buffered solutions for up to 12 hours under continuous irradiation. The test system was irradiated using a UV-filtered xenon lamp. The test system consisted of glass vials filled with *ca.* 20 mL of the treated pH 7 buffer solution. The vials were sealed, placed on a water-cooled steel block in the irradiation apparatus, and stirred with a magnetic stir bar. Volatiles were not measured. [¹⁴C]Residues were identified via one-dimensional TLC and HPLC co-chromatography and comparison of retention times with unlabeled reference standards. [¹⁴C]Residues were quantified via HPLC. Dark controls were not prepared in the definitive study, but chlorothalonil was stable in the dark control for the 96 hour preliminary study.

[¹⁴C]Chlorothalonil declined from 100.7% of the applied radioactivity at 0 hours posttreatment to 53.2% at 6 hours to a final of 20.9% at 12 days (study termination). Eight transformation products, four of which were considered major, were observed.

Based on first-order linear regression analysis using all data points, the **calculated half-life** of [¹⁴C]chlorothalonil in the irradiated solution was 7.1 hours (continuous irradiation; or 14.2 hours based on 12-hour light/12-hour dark cycles).

The **phototransformation half-life** for chlorothalonil at pH 7 is 14.2 hours, based on 12-hour light/12-hour dark cycles. The **calculated predicted environmental phototransformation half-life** of chlorothalonil in the irradiated samples is approximately 20.6 hours in the pH 7 buffer solution (10.3 hours based on continuous summer sunlight at 30° North Latitude).

Study Acceptability: This photodegradation study conducted using pH 7 sterile buffer solutions is classified as **acceptable**. It is scientifically valid, and can be used to fulfill the requirement for a photolysis in water study. While there were some minor deficiencies in this study, they have not effected the interpretation of the reported data.

Aerobic Aquatic Metabolism 162-4 (MRID 45908001)

The biotransformation of [phenyl-U-¹⁴C]-labeled 2,4,5,6-tetrachloro-1,3-benzenedicarbonitrile (chlorothalonil) was studied in running ditch water-clay sediment, and pond water-clay loam sediment systems from the United Kingdom for 100 days under aerobic conditions in darkness at 20°C. [¹⁴C]chlorothalonil was applied at a nominal rate of 0.83 mg a.i./L. The sediment:water ratios used were 1:2.7 for the ditch water-clay systems and 1:1.3 for the pond water-clay loam systems. The water-sediment systems were pre-incubated *ca.* 1 month. Water layers and

sediment extracts were analyzed for [^{14}C]chlorothalonil and its transformation products by reverse-phase HPLC. Four nonvolatile transformation products were identified. Trichloro-1,3-dicyanobenzene was tentatively identified through TLC co-chromatography. 2,4,5-Trichloro-6-mercapto-isophthalonitrile was identified via LC/MS, 4-hydroxy-2,5,6-trichloro-1,3-dicyanobenzene via HPLC and LC/MS, and 2,5,6-trichloro-1,3-dicyanobenzene-4-sulphonate (or positional isomer) is a proposed structure based on LC/MS.

For both test systems, conditions in the water layers of the treated systems were moderately reducing to moderately oxidizing, whereas conditions in the sediment layers were reducing to strongly reducing.

In the ditch water-clay sediment systems, chlorothalonil appeared to degrade rapidly with an observed half-life in the total system of <6 hours. Based on nonlinear/normal (2-parameter, unweighted) regression analysis, [^{14}C]chlorothalonil dissipated in the water layer and total system with calculated half-lives of 2.6 and 3.3 hours, respectively, with an observed DT_{50} in the sediment of 2-7 days.

In the pond water-clay loam sediment systems observed dissipation half-lives were <7 days total system.

Four major nonvolatile transformation products, trichloro-1,3-dicyanobenzene, 2,4,5-trichloro-6-mercapto-isophthalonitrile, 4-hydroxy-2,5,6-trichloro-1,3-dicyanobenzene and 2,5,6-trichloro-1,3-dicyanobenzene-4-sulphonate were detected in both systems. No minor products were identified. Two unidentified [^{14}C]compounds were detected as major products in both systems. In general, the levels of nonvolatile products were similar in the two test systems.

Results Synopsis:

Test system used: Running ditch water-clay sediment from United Kingdom.

Linear half-life (0- to 100-day data) in water: 16.8 days ($r^2 = 0.5254$).

Linear half-life (0- to 100-day data) in total system: 21.0 days ($r^2 = 0.4450$).

Major transformation products:

-Trichloro-1,3-dicyanobenzene (maximum of 24.0% in total system).

-2,4,5-Trichloro-6-mercapto-isophthalonitrile (maximum of 14.1% in sediment only).

-4-Hydroxy-2,5,6-trichloro-1,3-dicyanobenzene (maximum 16.2% in total system).

Minor identified transformation products:

-2,5,6-Trichloro-1,3-dicyanobenzene-4-sulphonate.

Test system used: Pond water-clay loam sediment from United Kingdom.

Linear half-life (0- to 100-day data) in water: 13.2 days ($r^2 = 0.6706$).

Linear half-life (0- to 100-day data) in total system: 13.4 days ($r^2 = 0.6699$).

Major transformation products:

-Trichloro-1,3-dicyanobenzene (maximum of 28.3% in total system).

- 2,4,5-Trichloro-6-mercapto-isophthalonitrile (maximum of 18.7% in total system).
- 2,5,6-Trichloro-1,3-dicyanobenzene-4-sulphonate (or its positional isomer; maximum of 10.4% in total system).

Minor identified transformation products:

- 4-Hydroxy-2,5,6-trichloro-1,3-dicyanobenzene.

Study Acceptability: This study is classified as **supplemental**. This study, conducted with [phenyl-U-¹⁴C]chlorothalonil, can not be used to fully meet the requirement for an aerobic aquatic metabolism study because the stability of parent chlorothalonil and its degradates during storage prior to analysis was not addressed.

Bioaccumulation in Fish 165-4 (MRID 45710224)

The bioaccumulation of [benzonitrile-U-¹⁴C]2,4,5,6-tetrachloro-1,3-benzenedicarbonitrile (chlorothalonil) was studied in rainbow trout (*Oncorhynchus mykiss*) at nominal concentrations of 0.1 and 0.5 µg/L under flow-through aquarium conditions. The test system consisted of three 150-L glass aquaria fitted with overflows to maintain a volume of 100 L at a loading rate of 70 fish per vessel. One low-dose and one high-dose aquaria were treated. A third aquarium was untreated and served as a solvent control. The exposure period lasted 28 days, and the subsequent depuration period lasted 21 days. During 28 days of exposure, the pH of the water was 7.0-7.6, the dissolved oxygen was 6.0-10.7 mg/L, and the temperature was 9-15°C. During the 21 days of depuration, the pH of the water was 7.2-7.6, the dissolved oxygen was 9.1-10.3 mg/L, and the temperature was 12-15°C. Water and fish tissue extracts were analyzed for [¹⁴C]chlorothalonil and its transformation products using normal and reverse phase one-dimensional TLC and HPLC, and were identified by comparison to reference standards of chlorothalonil and its transformation products.

In fish exposed at 0.1 µg/L, the calculated bioconcentration factors (BCF) are 256, 5812, and 3077 for the edible, non-edible, and whole fish tissues, respectively. After 1 day of depuration, total [¹⁴C]residues in whole fish tissues had decreased by 31% from the 28-day exposure values. The calculated depuration half-lives ($t_{1/2}$) are 13, 7.7, and 8.0 days for edible, non-edible, and whole fish tissues, respectively. [¹⁴C]Residues in the fish during exposure and depuration were not characterized.

In fish exposed at 0.5 µg/L, the calculated bioconcentration factors (BCF) are 306, 5694, and 3041 for the edible, non-edible, and whole fish tissues, respectively. In the edible and non-edible tissue (viscera and skeleton), [¹⁴C]chlorothalonil was not detected during the 28 days of exposure. In the edible tissue, two transformation products were identified. Three transformation products were identified in the edible tissue: the triglutathione conjugate was 9.1% of the recovered, the diglutathione conjugate was 18.8%, and 4-hydroxy-2,5,6-trichloro-1,3-dicyanobenzene was 3.9% of the recovered.

The calculated depuration half-lives ($t_{1/2}$) are 9.4, 7.0, and 7.1 days for edible, non-edible, and whole fish tissues, respectively.

Study Acceptability: This study is classified as **acceptable**. The study is scientifically valid, and can be used to fulfill guideline requirements for bioaccumulation in fish.