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GDCh-Advisory Committee
on Existing Chemicals of
Environmental Relevance (BUA)

1,2,3-Trichloropropane

BUA Report 154

(December 1993)



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Foreword

The German Chemicals Act (Chemikaliengesetz - ChemG) of 1980 stipulates that certain existing chemicals must be reported to the competent authority, if they exhibit properties which indicate that they may be hazardous, either alone or in combination with other substances.

In the summer of 1982, an Advisory Committee on Existing Chemicals of Environmental Relevance (BUA) was set up by the German Chemical Society (Gesellschaft Deutscher Chemiker - GDCh). It brings together representatives from the scientific community, the chemical industry and the governmental authorities. This Advisory Committee is responsible for elaborating appropriate solutions for substances of relevance for health and the environment on the basis of voluntary measures. It selects and examines existing chemicals from the aforementioned angles. The testing and evaluation are based on scientific criteria alone.

It was, therefore, necessary to develop priority setting procedures. In a first phase reports were only prepared for priority chemicals. Within the framework of a first priority setting procedure, chemicals were compiled from several priority lists and 135 chemicals were selected for detailed substance reports.

In a second priority setting procedure the survey of the German Chemical Industry Association (VCI) on all substances with a production volume of more than 10 tons per year was used as a starting list. Since this survey covered 4,600 chemicals, BUA decided to process the corresponding list in several stages. The first stage included approx. 1,050 substances with a production volume of more than 1,000 tons per year.

Detailed reports are drawn up on chemicals suspected of having a hazard potential and abridged reports on those presenting only a minor hazard potential, according to the current state of knowledge.

The detailed BUA reports take in both the published literature and data from industry. If data for the evaluation of the chemicals are not available, additional studies are recommended and the results are published as updates to the reports. The reports serve as a basis for the instigation of administrative measures, when there are indications of risks to health or the environment.

Tübingen, May 1993

Ernst Bayer
Chairman of the Advisory Committee
on Existing Chemicals
of Environmental Relevance

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BUA Report on

Summary and conclusions

Ecological aspects

Occurrence and distribution in the compartments

1,2,3-Trichloropropane (1,2,3-TCP) can be produced by the addition of chlorine to allyl chloride or by catalytic chlorination of 1,2-di-chloropropane. In the Federal Republic of Germany, 1,2,3-TCP is not intentionally produced. In the production of epichlorohydrin about 4 % 1,2,3-TCP is yielded as by-product. 1,2,3-TCP also occurs as a by-product in the production of vinyl chloride, 1,2-dichloroethane, propylene oxide and glycerin.

1,2,3-TCP also occurs as a by-product in nematicides containing 1,2-dichloropropane and 1,3-dichloropropene.

About 6,240 tonnes of 1,2,3-TCP were produced as by-product in the Federal Republic of Germany in 1990, of which 3,430 tonnes came from the production of epichlorohydrin. In the same year, 500 tonnes of 1,2,3-TCP were exported, while 5,740 tonnes were disposed of in incinerators for chemical residues. There are only marginal differences in the figures for 1991 and 1992.

No information is available on manufacturers of 1,2,3-TCP or on its production as a by-product in the former German Democratic Republic (GDR).

1,2,3-TCP can serve as a solvent for oils, fats, waxes, chlorinated rubber, natural and synthetic resins, as well as a paint and varnish remover and degreasing agent.

In addition, 1,2,3-TCP is used in 95 % of polysulphide production, in the synthesis of hexafluoropropylene, and as a trifunctional cross linking agent, i.e. for polysulphide elastomers. However, the abovementioned uses are not applicable to the Federal Republic of Germany. Significant emissions of 1,2,3-TCP into the atmosphere from the production and processing are not to be expected.

Emissions into the hydrosphere are about 102 kg/a. No data are available on emissions into the geosphere or biosphere. Emissions of 1,2,3-TCP via waste do not occur.

Emissions from the processing/use of epichlorohydrin, propylene oxide and glycerin, which contain residual amounts of 1,2,3-TCP, cannot be quantified, likewise the emissions from the use of 1,2-dichloroethane as a scavenger in leaded, carburetting fuels and as a solvent.

X

1978, in the German city of Bochum, random samples of air were found to contain $\leq 0.4 \mu\text{g}$ 1,2,3-TCP/ m^3 in 1984, $< 0.06 - 17.3 \text{ mg}$ 1,2,3- TCP/ m^3 were detected in the interior air of a United States' chemical plant.

A 1,2,3-TCP concentration of $0.03 \mu\text{g/l}$ was determined in an un filtered sample of sea water taken at a depth of 3 m from Scheldt Bay on the Dutch-Belgium border (buoy 87).

In 1984, 1,2,3-TCP concentrations of $0.4 - 0.6 \mu\text{g/l}$ were found in the rivers Emscher and Lippe, while in other Rhine tributaries and in the Rhine itself $\leq 0.1 \mu\text{g/l}$ were detected.

Between 1986 and 1989, the highest concentration of 1,2,3-TCP detected in the Rhine and its tributaries was $0.1 \mu\text{g/l}$.

In 1991, mean monthly concentrations of $0.1 - 0.4 \mu\text{g/l}$ were detected in the Rhine at Hagestein.

In 1980, 1,2,3-TCP concentrations between 0.02 and $4.2 \mu\text{g/l}$ were found in the rivers Leine, Weser and Elbe. In 1981/82, concentrations ranged from $< 0.02 - 0.1 \mu\text{g/l}$.

In analyses of Rhine sediment (between Rhine-km 639.1 and 863.8), 1987/88, at a detection limit of $1 \mu\text{g/kg}$, 1,2,3-TCP was not detected. From January to July 1977, the concentration of 1,2,3-TCP found in the tap water of 100 West German cities did not exceed $0.1 \mu\text{g/l}$.

A mean daily intake of $7.4 \mu\text{g/person}$ was determined from about 500 samples taken between 1977 and 1981 from a selection of food stuffs most commonly eaten in the Federal Republic of Germany (no further details).

No natural sources of 1,2,3-TCP are known.

On account of its physicochemical properties, 1,2,3-TCP is considered to be a substance which is volatile from water. In soil, a high mobility of 1,2 is to be expected.

Degradability

1,2,3-TCP is not readily biodegradable (modified MITI test).

Suspensions of nitrifying bacteria effected only 9 % elimination of 1,2,3-TCP after 24 hours incubation, while 23 % elimination was effected when NH_3 was added to the nutrient medium. There is evidence for potential elimination of 1,2,3-TCP by adapted, dechlorinating

microorganisms of the group *Actinomyces*. No data are available on degradation products. Hydrolytic degradation of 1,2,3-TCP in demineralized water is negligible (calculated half-lifetime at 25 °C: 44 and 74 years).

For 1,2,3-TCP emitted into the atmosphere, degradation through reaction with photochemically formed OH-radicals is possible. A half lifetime of 27.2 days has been calculated for 1,2,3-TCP in the atmosphere.

The half-lifetime for the photochemical degradation of 1,2,3-TCP in demineralized water was found to be far greater than 14 hours.

Accumulation

The experimentally determined n-octanol/water partition coefficient $\log P_{OW}$ of 2.27 indicates a moderate degree of bioaccumulation for 1,2,3-TCP. However, the experimentally determined bioconcentration factor (BCF) of 5 - 13 suggests that 1,2,3-TCP is subject to only weak bioaccumulation.

A soil sorption coefficient K_{OC} of 642, calculated from the n-octanol/water partition coefficient ($\log P_{OW}$) is indicative of a moderate to elevated degree of sorption to soil, while experimentally determined K_{OC} values of 95 (silty clay soil) and 77 (sandy clay soil) suggest very low to weak sorption to soil.

In view of the experimentally determined soil sorption coefficients no significant degree of geoaccumulation is to be expected.

Ecotoxicology

For aerobic, heterotrophic bacteria from the activated sludge of a wastewater treatment plant, a 15-h IC_{50} of 290 mg 1,2,3-TCP/l has been determined (test parameter: inhibition of oxygen uptake), while for *Nitrosomonas* (from activated sludge used in wastewater treatment in the meat processing industry) a 24-h IC_{50} of 30 mg/l was found (test parameter: inhibition of ammonia consumption). For methanogenic bacteria (from an enriched laboratory culture), a 48-h IC_{50} of 0.63 mg/l was determined (test parameter: inhibition of gas production). In a 3-h assimilation test with the green algae *Chlamydomonas angulosa* and *Chlorella vulgaris*, EC_{50} values of 112 and 170 mg/l, respectively, were determined (based on nominal concentrations).

Tests of the acute toxicity of 1,2,3-TCP towards aquatic invertebrates produced 48-h LC₅₀ values of 20 and 35 mg for the water flea, *Daphnia magna*. For the amphipod, *Chaetogammarus marinus*, a 48-h LC₅₀ of 60 mg/l and a 96-h LC₅₀ of 45 mg/l were determined.

A NOEC (no-observed-effect concentration; based on immobilization) of 4 mg/l was calculated for *Daphnia magna* using the quantitative structure activity relationship (QSAR). In respect to reproduction toxicity, an EC₅₀ of 6.4 mg/l was calculated for the water flea, *Daphnia magna*.

In respect to the chronic toxicity of 1,2,3-TCP, the following results were obtained from a semistatic bottle test with the amphipod *Chaetogammarus marinus*: 7-day LC₅₀ of 33 mg/l; 14-day LC₅₀ of 22 mg/l; 21-day LC₅₀ of 20 mg/l.

In tests of acute toxicity towards the bluegill sunfish, *Lepomis macrochirus*, 24-h, 48-h and 96-h LC₀ values of ≥ 56 mg/l and a 24-h LC₁₀₀ of ≤ 100 mg/l were determined. The 96-h NOEC is given as 10 mg/l (static test; nominal concentrations).

In an acute toxicity test of 1,2,3-TCP towards the rainbow trout, *Oncorhynchus mykiss*, formerly *Salmo gairdneri*, the following results, based on nominal concentrations of 10, 18, 32, 56 and 100 mg/l were obtained: a 24-h LC₅₀ of 75 mg/l; a 48-h LC₅₀ of 64 mg/l and a 96-h LC₅₀ of 42 mg/l; a 96-h NOEC of < 10 mg/l is given (static test; with feeding). While 1,2,3-TCP concentrations of up to 32 mg/l caused no mortalities, concentrations of 56 and 100 mg/l resulted in 100 % mortality after 96 and 24 hours, respectively.

In respect to the acute toxicity of 1,2,3-TCP towards the fathead minnow, *Pimephales promelas*, a 96-h LC₅₀ of 66.5 mg/l and a 96-h EC₅₀ of 65.0 mg/l have been determined (based on effective concentrations).

In an extended test of toxicity towards 2 - 3 month old guppies, *Poecilia reticulata*, an LC₅₀ of 41.6 mg/l was obtained (semistatic test; nominal concentration).

The effect of 1,000 mg 1,2,3-TCP/kg soil (nominal concentration) on the respiration of soil microorganisms was studied in silty clay soil (carbon content: 1.43 - 1.55 %) and in sandy clay soil (carbon content: 0.62 - 0.70 %). The higher rate of microbial respiration was found for the silty clay soil. Measurement of CO₂ production after 4 days showed that in silty clay soil 1,2,3-TCP reduced respiration by 0.09 mg/kg soil/hour, while in sandy clay soil respiration

was reduced by 0.18 mg/kg/hour. Daily measurements of CO₂ production showed a reduction in respiration in both types of soil. However, after 6 days there was no longer any significant difference in respiration rate between either soil type and the controls.

Toxicological aspects *)

Following oral administration, 1,2,3-TCP is rapidly absorbed and distributed in the tissues. Distribution studies with radiolabelled 1,2,3-TCP show the highest concentrations in the liver and kidneys, whereby radioactivity was mainly bound to macromolecules (proteins, DNA, RNA). Following oral administration to rats, 1,2,3-TCP is metabolized, presumably via conjugation with glutathione, particularly to N-acetyl-S-(3-chloro-2-hydroxypropyl)-L-cysteine and S-(3-chloro-2-hydroxypropyl)-L-cysteine.

In vitro studies with rat and human liver microsome fractions have shown that 1,2,3-TCP can be metabolized to the directly acting mutagen, 1,3-dichloroacetone.

Following oral administration, 1,2,3-TCP is eliminated mainly in the urine. 90 % of the administered dose of radiolabelled 1,2,3-TCP were eliminated within 60 hours in the urine, faeces and exhaled CO₂.

The values obtained for acute toxicity (LD₅₀) in rats following oral administration are between 99 and 555 mg/kg body weight, and following dermal application to rats and rabbits, between 250 and 2,457 mg/kg body weight. 4-h LC₅₀ values of ca. 3,000 mg/m³ were obtained for inhalation exposure of mice and rats. The symptoms of intoxication are characterized by dyspnoea, irritation of mucous membranes, ataxia and general sedation, as well as by liver and kidney damage.

Direct contact of 1,2,3-TCP with the skin causes slight to strong irritation, while direct contact with mucous membranes results in moderate irritation.

In various tests with guinea pigs, 1,2,3-TCP showed no or only a very slight sensitising effect.

The target organs of 1,2,3-TCP toxicity following repeated admin-

*) See Annex: Toxikologisch-arbeitsmedizinische Begründungen von MAK-Werten (1993)

istration are the liver and kidneys. Necrosis and hypertrophy of hepatocytes are given particular mention in respect of pathological changes to liver. Kidney damage is observed in the form of tubular hyperbasophilia, regenerative hyperplasia and proteinaceous tubular casts. Following inhalation exposure to 1,2,3-TCP, the main symptom was marked irritation of the nasal mucosa.

After just 90 days oral administration of 1,2 to rats, indications of proliferative and neoplastic changes were observed in the form of adenocarcinoma of the mammary gland, forestomach squamous cell hyperplasia and bronchoalveolar adenoma.

In the 90-day feeding study, the NOEL for rats was 1.4 mg/kg body weight/day and for mice, 16 mg/kg body weight/day. In a 90-day test of inhalation exposure with rats (6 hours a day, 5 days a week), a NOEC of 9.4 mg/m³ was determined.

In vitro, 1,2,3-TCP is both mutagenic and clastogenic, but only following metabolic activation. In rats, *in vivo*, 1,2,3-TCP had a damaging effect on liver and kidney DNA, but did not cause dominant lethal mutations. In the micronucleus test with mice and the UDS test with rats, no indication of a genotoxic effect was found. Studies with rats (whole body exposure) provided evidence of 1,2,3-TCP having an aneuploidy inducing effect.

In long-term gavage studies, 1,2,3-TCP has been found to be carcinogenic in mice and rats, numerous neoplastic changes being observed to occur in both species. After 2 years administration to rats, a significant, dose-dependent increase of the incidence of neoplastic changes was observed in the oral mucosa, forestomach, pancreas, kidney, preputial gland, clitoral gland and mammary gland. In male mice, a dose-dependent increase of the incidence of neoplastic changes of the forestomach, liver and Harderian gland, in female mice also of the oral mucosa and uterus, was found.

1,3-Dichloroacetone is suspected to be the reactive intermediate responsible for the toxic, mutagenic and carcinogenic effects of 1,2,3-TCP.

Studies of reproduction toxicity provide no indication of 1,2,3-TCP having an effect on fertility or having any embryotoxic or teratogenic properties.

In humans, inhalation exposure to 613 mg 1,2,3-TCP/m³ had an irritating effect on eyes and throat, but not on the nasal mucosa.

Recommendations

Ecology

The occurrence of 1,2,3-TCP in the environment, in food and in samples of human tissues cannot be adequately explained by the sources covered in this report.

However, available data on the ecotoxicology of 1,2,3-TCP and on its behaviour in the environment are considered adequate for an evaluation of 1,2,3-TCP's environmental relevance.

Toxicology

There is a lack of data in respect to the prenatal toxicity of 1,2,3-TCP. 1,2,3-TCP is a waste product which is placed in Group III A2 (carcinogenic in animals) of German MAK-list (list of maximum concentrations at the workplace). In view of the protective measures taken on account of this classification, further clarification of 1,2,3-TCP's prenatal toxicity is not required.