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

Acrolein

BUA Report 157
(December 1994)



S. Hirzel

Wissenschaftliche Verlagsgesellschaft 1996

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Committee on Existing Chemicals
of Environmental Relevance

Beratergremium für
Umweltrelevante Altstoffe (BUA)



S. Hirzel

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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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(2-Propenal)

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BUA Report on Acrolein

Summary and conclusions

Ecological aspects

Occurrence and Distribution in the Compartments

About 25 % of the amount of acrolein produced and isolated in 1991 in the Federal Republic of Germany were processed there. Approximately 75 % of the isolated acrolein were exported. About 2,000 t acrolein were imported in 1991 into the Federal Republic of Germany. Data about further imports are unavailable. Moreover, a maximum of 196,000 t acrolein/a (based on a total capacity of 252,000 t acrylic acid/a) is formed as an unisolated intermediate product during the manufacture of acrylic acid.

Acrolein is used exclusively as an intermediate in the Federal Republic of Germany. The main fraction, about 70 - 80 % of the acrolein¹⁾, is reacted to the amino acid D,L-methionine via the intermediate product methylmercaptopropionaldehyde (MMP). Approximately 15 – 25 % are processed to 3,4-dihydro-2-methoxy-2H-pyran which is subsequently reacted to glutaric dialdehyde. Respectively less than 5 % of the acrolein are further processed to 3-formyl-5,6-dihydro-2H-thiopyran (end product: thiopyran-3-aldehyde), to tetrahydrobenzaldehyde and to fragrances (Lyral). There is no known application area in the Federal Republic of Germany in which acrolein is directly used.

The emission of acrolein into the atmosphere (Federal Republic of Germany) during production was about 0.006 - 0.01 t/a in 1990 to 1992. There was no resulting emission into the hydrosphere. With the processing in the Federal Republic of Germany, about 0.006 t acrolein/a and about 6 t acrolein/a were released into the atmosphere and hydrosphere during the same period, respectively. An emission into the geo- and biosphere is unquantifiable. The far largest acrolein emissions into the environment (atmosphere) occur through automobile exhaust, i. e. about 2,806 - 11,124 t acrolein/a

1) based on the acrolein isolated and further processed in the Federal Republic of Germany

in 1992 in the Federal Republic of Germany, as well as through cigarette smoke, i. e. at least 30.5 - 248 t acrolein/a (main and side stream smoke, without particulate phase). Additional unquantifiable emissions occur through exhaust gases of stationary spark-ignition and diesel engines, through engines of other land-based vehicles (e. g. agricultural hauliers, military vehicles, diesel locomotives), inland ships and aeroplanes, through smoke from the incomplete combustion of wood, plastics and tobacco (beyond cigarettes) as well as from heating (overheating) of fat.

In some studies conducted in the vicinity of cities, acrolein could be detected in the atmosphere qualitatively (Toulon, France and Stockholm, Sweden) and quantitatively (Sao Paulo and Salvador, Brazil as well as Stockholm, Sweden), whereby the measurement values nearby high-traffic roads were highest (up to 27 $\mu\text{g}/\text{m}^3$). However, acrolein was undetectable (detection limit: 35 and 1.65 $\mu\text{g}/\text{m}^3$ in some other measurements (Californian coast, Baton Rouge, Newark and Plainfield, U.S.A.).

In one study, acrolein was detected together with acetone (analytically unseparated) in a concentration of 0.5 $\mu\text{g}/\text{m}^3$ (open sea) and 2.3 $\mu\text{g}/\text{m}^3$ (coastal region) in one clean air area in the U.S.A. However, no statement was made about the ratio of acrolein/acetone.

Concentrations of up to 448 μg acrolein/l liquid could be detected in fog samples in Italy during one monitoring program (3 months).

Acrolein has likewise been detected in indoor areas. In one restaurant (U.S.A., 5 - 25 persons present, mostly smokers), concentrations of 21 - 24 $\mu\text{g}/\text{m}^3$ were measured. The acrolein concentration in one living room (U.S.A.) was 0.8 - 4.5 $\mu\text{g}/\text{m}^3$ whereby the measured values were attributed to a leaky wood stove. In another study in the Netherlands, no acrolein could be detected in 6 different living rooms (detection limit: 5 $\mu\text{g}/\text{m}^3$).

Acrolein in concentrations of 5 - 11 $\mu\text{g}/\text{l}$ could be detected in 3 of 4 unidentified rain water samples.

Acrolein could be detected qualitatively in some few samples of disposal site ground water (9 samples of 7 landfills, 479 different landfills in total) in the U.S.A. There were 270 μg acrolein/l found in one of five leachate samples of a municipal waste landfill, likewise in the U.S.A., while no acrolein could be found in the other samples (detection

limit unspecified). In contrast, no acrolein could be detected in various water samples taken from the area of one former industrial waste site in the U.S.A. (detection limit: 1 and 100 µg/l).

Nineteen of 1,265 samples of American industrial waste waters contained detectable acrolein concentrations. In surface waters, however, acrolein could be detected in only 2 of 798 water samples (evaluation of one U.S. EPA data bank). Acrolein was undetectable in 22 samples of ground water and waste water of one American plastic manufacturer (detection limit: 10 µg/l) as well as in 3 ground water samples (48 - 55 m below the surface) of an area supposedly contaminated with fuels (detection limit: 5 µg/l).

None of 331 sediment samples from the U.S.A. contained detectable acrolein concentrations (evaluation of a U.S. EPA data bank). Acrolein in a concentration of 58 µg/kg soil (dry/wet weight unspecified) could be detected (detection limit: 10 µg/kg) in one of 30 soil samples taken in a depth of about 12 m on a fire-fighter-training site in the U.S.A.

Acrolein was found in biological material (not further specified) in one of 87 samples (evaluation of a U.S. EPA data bank).

Acrolein could be detected in numerous foodstuffs:

in newly prepared beer (≤ 2 µg/l), aged beer (≥ 5 µg/l), wines, spoiled wine (14 mg/l), brandies, "peppery" rums, whiskies, apple eau-de-vie, ethyl alcohol of various origin (0.2 - 0.4 mg/l), heated and aged animal fats, vegetable oils, bread (3 different types), white bread, fried baking powder- and yeast doughnuts (0.1 - 0.9 mg/kg), ripe tomatoes, cooked potatoes, raw chicken breast muscle, turkey meat, sour salted pork, cooked horse mackerel and in the bread crumb layer of cod filets (up to 0.1 mg/kg). Acrolein was found in one of 4 samples of air over stored milk. It was likewise detected as a thermal degradation product of amino acids during the cooking process.

Acrolein can occur in mammalian tissues as a degradation product of polyamines, such as e. g. spermidin. The enzyme polyaminoxidase, present in phagocytes (macrophages), is primarily active here.

In 2 different model tests in closed flasks for detecting the formation of acrolein through UV-irradiation of arachidonic acid (UV-wave length: $\lambda = 360$ nm) and triolein

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($\lambda = 300$ nm), acrolein could be detected in concentrations of 2.5 $\mu\text{g}/\text{mg}$ arachidonic acid and 59 ng/mg triolein.

By means of heat-treated methanol yeast cells *Candida boidinii* S2, a maximum yield of 3 % acrolein could be obtained after 2 hours in one model test with 5 % allyl alcohol as the substrate.

Based on the established Henrys Law constant, a transport of acrolein, released into surface water, from water into the air is expected through evaporation.

Acrolein shows only low sorption to soil. Thus, the substance is moderately high to highly mobile in soil and can be leached out into ground water or released into the atmosphere. There are indications that the fraction of acrolein adsorbed to soil is no longer capable of being eluted by solvents (irreversible process).

Degradability

A biodegradation of acrolein takes place only with adapted micro-organisms. Thus, biodegradation is expected neither in soil nor in the hydrosphere.

Acrolein does not possess any hydrolyzable groups. Nevertheless, in the presence of water, the reversible addition of a water molecule onto the C-C double bond (hydration) to 3-hydroxypropanal (HPA) takes place. At every reaction time, the HPA formed from acrolein exists in equilibrium with acrolein as well as with its dimer and its hydrate. Besides this, in a subsequent reaction of HPA with acrolein, 4-oxa-1,7-heptanedial (3,3'-oxydipropionaldehyde) is formed which reacts to further by-products. Equilibrium at 20°C lies to ca. 91.0 - 95.5 % on the side of HPA in neutral, acidic, buffered as well as in alkaline solutions. Studies with natural, unsterilized water samples show, however, that acrolein completely reacts to HPA. Half-lives of 15 hours were found in waste water, while those of 29 - 61 hours and 257 hours (11 days) were established in drinking water and in distilled water, respectively. In one field test (irrigation channels), the half-life was only 4.3 hours, whereby this considerably lesser time span was attributed to evaporation processes, turbulence and adsorption effects. Less significant for the degradation in shallow surface water are photolysis and the

reaction with OH-radicals.

The stability of acrolein in the atmosphere is limited by the rapid gas phase reactions with the hydroxyl radical and ozone. Other degradation pathways are the reaction with the nitrate radical (nighttime) as well as photolysis (daytime) which is less significant. Likewise described, but of lesser importance, is the degradation by the reaction with atomic oxygen ($O(^3P)$). The half-life of acrolein in the troposphere is less than one day (ca. 9 - 24 hours) for the reaction with the OH-radical, ca. 2 - 28 days for the reaction with the ozone molecule and ca 5 - 11 days for the reaction with the nitrate radical. The half-life of the photolysis of acrolein in the troposphere is 10 days in the lower troposphere (sea level; solar zenith angle: 40°) and is less than 5 days in the upper troposphere (263 hPa 10 km altitude).

Accumulation

A bioaccumulation of acrolein is not expected on the basis of the established octanol/water partition coefficients ($\log P_{OW} = -1.10$ to 1.02). The bioaccumulation factor of 344 determined with radioactive labeled acrolein is presumably not attributable to the bioaccumulation of acrolein per se but rather to the incorporation of radioactive labeled carbon into the tissue, for example as the result of the formation of acrolein metabolites.

Ecotoxic Effects

The listed effective concentrations in the aquatic medium are nominal values, if not otherwise specified. The actual substance concentration in the medium in these cases is lower due to the (moderately high) volatility as well as the hydration of acrolein.

An initial inhibition of the cell reproduction of *Pseudomonas putida* could be found after exposure for 16 - 18 hours to acrolein concentrations of 0.21 - 0.33 mg/l. A 16 h IC_{10} value of 0.04 mg acrolein/l was determined in the growth inhibition test for the blue

algae/cyanobacterium *Microcystis aeruginosa*.

With regard to the biomass, an EC₅₀ value of 0.026 mg acrolein/l was determined for the green algae species *Scenedesmus subspicatus* after an exposure period of 72 hours. The NOEC, considering the growth rate, was 0.01 mg acrolein/l.

Acrolein in a concentration of 2 - 5 mg/l was used in one open-field test on the suppression of growth of the pond-weed (*Potamogeton striatus*) in an irrigation canal. Within a period of > 24 hours, the biomass of *P. striatus* was reduced by 30 - 50 % on a 7 - 10 km distance of the canal system.

A 48 h EC₅₀ value of 0.022 mg/l, determined in a flow-through system, is available on the acute toxicity to the water flea (*Daphnia magna*).

In one chronic toxicity study over a period of 3 generations (64 days) of a daphnia population (water flea, *Daphnia magna*), the MATC (maximal acceptable toxicant concentration) for reproductive toxic effects in the 2nd and 3rd generation ranged from 0.0169 mg/l to 0.0336 mg/l. In the 1st generation, the reproductive rate was reduced compared to the controls at an exposure of 0.0336 mg/l.

For mussels of the species *Dreissena polymorpha*, a LC₅₀ value of 4.9 mg/l could be ascertained in a semi-static test after a 14-day exposure period. One study in the toxicity of acrolein in a flow-through system on the American oyster (*Crassostrea virginica*) resulted in an EC₅₀ (96 h) value of 0.055 mg/l based on the growth of the shell.

For the rainbow trout (*Oncorhynchus mykiss*) and the fathead minnow (*Pimephales promelas*), LC₅₀ values of 0.016 mg/l and 0.014 mg/l, respectively, were determined in studies on the acute toxicity of acrolein after an exposure period of 96 hours. A 96 h LC₅₀ value of 0.007 mg/l could likewise be determined in the flow-through System for tadpoles of the frog (*Xenopus laevis*).

In a study of the toxicity of acrolein in the yeast *Cryptococcus neoformans*, 30 % of the *C. neoformans* cells died after a 2 hour incubation period at a concentration of 0.56 mg acrolein/l. The death rate was 95 % at a concentration of 5.6 mg/l.

Acrolein in a concentration of 1.4 mg/m³ damages the leaves of higher plants (*Spinacia oleracea*/spinach, *Cichorium endivia*/endive, *Beta sp.*/sugar beet) after an exposure period of 3 hours in the fumigation chamber. No toxic effects occurred after a

9 h exposure period at a concentration of 0.23 mg/m³.

A dose of 100 mg acrolein/kg body weight did not lead to any toxic findings in 2 starlings (*Sturnus vulgaris*).

After an exposure period of 20 minutes, the toxic threshold for the cilia activity of the tracheal epithelium in the sheep (*Ovis sp.*; *in vitro* test) was specified to be 35 - 47 mg acrolein/m³ as well as 47 mg acrolein/m³ for the bronchomotoricity in the guinea pig (*Cavia sp.*; *in vivo* test).

Toxicological Aspect

The high reactivity of the acrolein molecule is the reason that it is primarily bound locally to the application site. After absorption in the gastrointestinal tract, the main pathway of biotransformation is described to be the conjugation with glutathione with subsequent oxidation or reduction of the aldehyde group. Acrylic acid as well as the reactive metabolites glycidaldehyde and glycerinaldehyde, formed by oxidation of the double bond, could only be detected in *in vitro* tests with microsomal fractions after induction of cytochrome P-450-dependent monooxygenases.

The LD₅₀ values for rats after oral uptake lie between < 11 and 46 mg acrolein/kg. The LD₅₀ value after dermal application of a 20 % aqueous acrolein solution to the rabbit is 335 mg/kg, while undiluted acrolein shows a LD₅₀ value of 562 mg/kg. The LC₅₀ values for the inhalative exposure of the rat with acrolein lie at about 0.02 mg/l/4 h. After inhalation of acrolein, concentration-dependent pronounced effects on the respiratory tract (nasal irritation, dyspnoea) occur because of the local irritation.

Acrolein is strongly irritating to skin and mucous membranes even in highly diluted solutions. Therefore pure acrolein is considered corrosive. Acrolein did not reveal a sensitising potential in animal experiments.

Subacute inhalation in rats and mice leads to irritation with inflammation, ulceration, necrosis, as well as metaplastic, hyperplastic and dysplastic alterations of the respiratory and olfactory epithelium.

Irritation and inflammation with hyper- and metaplastic changes in the respiratory tract are also the primarily observed effects in subchronic and chronic inhalation studies in various species. At higher dosages, inflammatory changes in the liver and kidney also occur. A concentration of 0.9 mg/m^3 (13 weeks, 6 h/d, 5 d/w) was proven to be the NOEL in the hamster and rabbit. In the rat, however, a concentration of 0.9 mg/m^3 caused damage to the nasal mucosa after 90 days but not after 62 days of exposure. The NOEL for the rat was 0.15 mg/m^3 with continuous exposure (24 h/d, 7 d/w) for 61 days.

After chronic oral administration, reduced body weight gain, increased mortality and changes of clinical-chemical parameters were observed at high dosages. Pathological organ changes, however, were not observed. The NOEL for rats and dogs is 0.5 mg/kg and is 2.0 mg/kg for mice.

Acrolein reacts with nucleic acids and inhibits their synthesis. Tests for primary DNA damage and sister-chromatid exchange are partially positive. Positive and negative results have been obtained in various test systems with bacteria, yeast and mammalian cells. In these test systems acrolein shows mildly genotoxic properties mainly in the range of cytotoxic and bacteria-toxic concentrations. *In vitro* chromosome aberration tests are mostly negative. *In vivo* studies on mutations on *Drosophila* yield contradictory results in various test protocols. *In vivo* studies in mammals, one chromosome aberration test in the rat and a dominant lethal test are negative. Difficulties in testing the genotoxic potential arise from the high cytotoxicity as well as from the high reactivity of acrolein. From the available studies, a mildly genotoxic property can be derived from some *in vitro* tests, while no mutagenic properties were noted in studies in mammals.

Acrolein is non-carcinogenic after oral and inhalative exposure. A co-carcinogenic effect on the skin is not observed after co-administration of acrolein and benzopyrene. Nevertheless, some of the performed studies (inhalative and dermal exposure) are inconclusive because of the low animal number or short test period.

Acrolein shows no adverse effects to reproduction and development after oral or inhalative exposure in animal experiments.

In humans irritation to the skin and mucosa of the eyes and the respiratory tract are the primarily observed effects.

Recommendations

Ecology:

The available data for acrolein on ecotoxicology and environmental behaviour are considered to suffice for an evaluation of the environmental relevance.

In the processing of acrolein by the BASF AG, about 6 t acrolein/a are directed into the treatment-requiring waste water. Because of the reactivity of acrolein, it is expected that a fraction of the acrolein is reacted in the complex waste water. Because corresponding data on the elimination capacity of the BASF waste water treatment plant are unavailable with respect to acrolein, studies (suitable analyses in sewage treatment plant effluent) on determining the elimination capacity must be performed.

Toxicology:

All toxicological end points are sufficiently examined.

No further tests are recommended for acrolein.