

Initial Risk Assessment of Acetanilide with Respect to Ecological Integrity

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아세트아닐리드의 초기 환경위해성 평가

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요 약

아세트아닐리드는 의약품과 염료의 합성과정에서 중간체로서 공기와 폐수를 통하여 환경 중에 방출될 수 있다. 아세트아닐리드는 호기적 조건하에서 신속히 생분해되고 OH 라디칼의 존재하에 간접적으로 광분해된다. 생물농축계수는 4.5로 추정되므로 수생생물에서의 생물농축은 낮을 것으로 예상된다.

아세트아닐리드에 관한 생태독성학적 데이터 조사결과 4종 어류에 대한 급성독성치만 보고되어 있으며, EUSES 시스템에 의하면 어류에서의 최저 PNEC 값(예상 무작용농도)은 0.01 mg/l이고 표면수에서의 PEC 값(예상 환경농도)은 지역수준에서 최악의 경우 9.1×10^{-5} mg/l이다. 지역수준에서 표면수에 대한 아세트아닐리드의 RCR(위해성지수)은 9.1×10^{-3} 으로 추정되어 어류에 대한 안전성은 충분하다. 그러나 국지 수준에서의 RCR은 물과 침적물에서 각각 1.3과 1.6이므로 제조공장 주변에서는 생태독성 위험이 존재할 것으로 추정된다.

아세트아닐리드의 환경위해성 평가를 보다 정확하게 하기 위해서는 물벼룩과 조류에 대한 급성독성 자료가 보완되어야 할 것이며, 따라서 이에 대한 실험이 진행되어야 할 것으로 사료된다.

INTRODUCTION

The investigation of the safety of the nearly 100,000 chemicals currently in commerce is a daunting global challenge that can only be met if approached in a systematic way. This enormous task has

been undertaken by the OECD, based on compilation, review and assessment of toxicity data on the environment and human health.

Through the 1990 OECD Council Decision, member countries have decided to undertake the investigation of high production volume (HPV) chemicals

in a co-operative way. These HVP chemicals include all chemicals reported to be produced or imported at levels greater than 1,000 tons per year in at least one member country. Member countries will co-operatively (1) select the chemicals to be investigated, (2) collect effects and exposure information of the chemical, (3) complete the agreed dossier for the Screening Information Data Set (SIDS) by testing, and finally (4) make an initial assessment of the potential hazard of each chemical investigated.¹⁾

Among chemicals selected for investigation by Korean side from the year of 1999, acetanilide is the first to collect pertinent information, review the data quality and attempt an initial risk assessment. This study was intended to make an initial ecological risk assessment of acetanilide following the OECD manual with limited data available at the moment. This case study is expected to trigger the attempt to identify, prioritize, and manage chemicals of environmental concern in the government, the industry, and the public. The word "initial" was used because the data used for the risk assessment are not complete set of data generated solely by experiment.

MATERIALS AND METHODS

1. Data search

All the data used in this study were the product scanned through the following four major data sources;

1) Worldwide database

Database	Data sources	
IUCLID	Hoechst AG Frankfurt/Main ACGIH Natl. Tech Inf. Ser H/B Chem. Phys.	
TOMES	CHRIS	REPROTEXT
	DOLPHIN	RTECS
	NAERG	SHEPARDS
	HAZARDTEXT	TERIS
	HSDB	OHM/TADS
	IRIS	INFOTEXT
	MEDITEXT	NJ HSFS
	NIOSH	ACROS MSDS by Fisher Scientific

2) International Organization

Database	Data sources
UNEP (irptc.unep.ch)	GEENET IRPTC PRTR Infoterra (DAIN-555 sites on env. chemicals)
WHO (193.51.164.11/cgi/HOUND/Chem)	GRID GINC Chem. DB Other Sites
ILO (www.ilo.org/public)	ICPS GEENET IARC
FAO (www.fao.org/WAICENT)	World Agriculture Inf. Ctr INCHEM by IPCS
OECD (www.oecd.org)	Exichem by Chemicals Program

3) National Organization

Database	Data sources	
USA (www.epa.gov/ecotox) (www.cdc.gov/niosh) (ntp-db.niehs.nih.gov)	EPA - 8 Triage Chem. studies DB - Cal EPA Dept. of Pesticide Reg. - Cal EPA Dept. of Pesticide Reg. - ECOSAR - Ecotox - Environfacts - IRIS - OPPT Chemical Factsheet - TRI Factsheet	
	CDC - HazDat by ATSDR - Int. Safety Cards - OSH Guidelines for Chem. Haz. - OSHA Pels - Pocket guide to Chem. Haz. - NIOSTIC DB	
	NIH - NIH Chem. Safety DB NTP - NTP's chemical compendium - NTP's chemical DB - Report on carcinogens	
	FDA	
	EU (eccdin.etomep.net) (ulisse.etoit.eudra.org/ECDIN/)	ECDIN EEA (EIONET) JRC ERIN (www.iarc.fr)
	CANADA	CCOHS : - CHEMINDEX - CHEMINFO - INCHEM - MSDS DB - OSH Ref. - RTECS
	JAPAN	NIHS - GINC by UNEP/ILO/OECD/ NIHS JETOC
	KOREA	KRPTC

4) Company, University & Others

Database	Data sources
Company	Chemfinder Ciba
	Dow Chem Eastman Chem
	GE Plastic Monsanto
	Safety Info. Resources
	MSDA Search Rohm and Haas
	Shell (US) Chem. Sumitomo
	Green Chemicals
University	Univ. Akron, Hazardous Chem. DB
	Stanford Univ., Chemical Safety Portfolio
	OSU - EXTTOXNET (ace.orst.edu/info/extoxnet)
	UC Davis (www.envtox.ucdavis.edu/DocCenter)
	- Agricola (www.nal.usda.gov/ag98)
	- Cancernet by NCI
	- CHRIS
	- EXTTOXNET
	- Federal Register
	- International Grateful Med by NLM
	- IRIS
	- Melvyl Catalog by UCAL
	- Nat.Tech. Inf. Svc
	- NIOSH Chem. OSH DB
	- PubMed by NLM
- TOXNET BY NLM	
Others	NLM - CCRIS
	- ECDIN
	- GENE Tox
	- Medline
	- Toxnet
	CAS - ACS's Chemical Abstract
- STN International	

2. Prediction of data

It was found that many data needed for the risk assessment were not available. Therefore, several programs were used for the prediction of the parameters. These were as follows:

- EUSES (European Union System for the Evaluation of Substances, Ver. 1.00)²⁾
- EPIWIN (EPIWIN v2.2, SRC-EPI for Microsoft Windows, 1994~1996)

RESULTS

1. Chemical identity and physicochemical properties

OECD Name : Acetanilide (CAS No. 103-84-4)

Synonyms : Acetaminobenzene; Acetanil; Acetanilid; Acetic acid anilide; Acetoanilide; Acetylaminobenzene; Acetylaminobenzol; Acetylaniline; Antifebrin; N-Acetyl aniline; N-Acetyl-benzenamine; N-Phenyl acetamide; N-Phenyl acetic acid amide; Phenalgen; Phenalgin; USAF EK-3

Structural Formula : $\text{CH}_3\text{CONHC}_6\text{H}_5$

Degree of Purity : >97% (industrial grade)

Physical-chemical properties ;

Melting Point : 114°C

Boiling Point : 305°C at 101.3 kPa

Vapour Pressure : 0.16 Pa at 25°C

Water Solubility : 4 g/l at 20°C

Log Pow : 1.16

Classification in member countries : Not classified as toxic chemicals in the Toxic Chemicals Control Act, Republic of Korea

2. Exposure

1) Estimated national production and import

Total production of acetanilide in Korea was about 2,300 metric tons/year and the import into Korea was less than 1% of the produced in 1998. Acetanilide is produced by one company in Korea. Data on production volumes in other countries are not available.

2) Use categories

Of the 2,300 tons consumed in Korea, most is used as an intermediate for the syntheses of pharmaceuticals and dyes. Less than 0.5 ton is used as a stabilizer in hydrogen peroxide solution. Most of the acetanilide is consumed by one company in Korea, which is the only producer of the chemical. Acetanilide is marketed as a solid form with the purity of >97% as industrial grade in Korea.

Table 1. Input data for the EUSES

Input items	EU TGD default values	Input values of this study	Unit
Release estimation			
Fraction of EU production volume for region	0.1	1	—
Fraction connected to sewer systems	0.7	0.6	—
Characteristics of compartments			
<i>General</i>			
Density of solid phase	2.5	2.5	kg/l
Density of water phase	1	1	kg/l
Density of air phase	1.3E-03	1.3E-03	kg/l
Environmental temperature	12	12	°C
Constant of Junge equation	0.01	0.01	Pa.m
Surface area of aerosol particles	0.01	0.01	m ² /m ³
Gas constant	8.314	8.314	Pa.m ³ /mol/°K
<i>Suspended matter</i>			
Volume fraction of solids in suspended matter	0.1	0.1	m ³ /m ³
Volume fraction of water in suspended matter	0.9	0.9	m ³ /m ³
Weight fraction of organic carbon in suspended matter	0.1	0.1	kg/kg
<i>Sediment</i>			
Volume fraction of solids in sediment	0.2	0.2	m ³ /m ³
Volume fraction of water in sediment	0.8	0.8	m ³ /m ³
Weight fraction of organic carbon in sediment	0.05	0.05	kg/kg
<i>Soil</i>			
Volume fraction of solids in soil	0.6	0.6	m ³ /m ³
Volume fraction of water in soil	0.2	0.2	m ³ /m ³
Volume fraction of air in soil	0.2	0.2	m ³ /m ³
Weight fraction of organic carbon in soil	0.02	0.02	kg/kg
<i>STP sludge</i>			
Fraction of organic carbon in raw sewage sludge	0.3	0.3	kg/kg
Fraction of organic carbon in settled sewage sludge	0.3	0.3	kg/kg
Fraction of organic carbon in activated sewage sludge	0.37	0.37	kg/kg
Fraction of organic carbon in effluent sewage sludge	0.37	0.37	kg/kg
Degradation and transformation rates			
Concentration of OH-radicals in atmosphere	5E+05	5E+05	molec/cm ³
Rate constant for abiotic degradation in STP	0	0	1/day
Rate constant for abiotic degradation in bulk soil	0	0	1/day
Rate constant for abiotic degradation in bulk sediment	0	0	1/day
Rate constant for anaerobic biodegradation in sediment	0	0	1/day
Fraction of sediment compartment that is aerated	0.1	0.1	m ³ /m ³
Sewage treatment			
<i>General</i>			
Number of inhabitants feeding one STP	1E+04	3E+05	eq
Sewage flow	200	300(527) [#]	l/eq/d
Temperature of air above aeration tank	15	15	°C
Temperature of water in aeration tank	15	15	°C
Height of air column above STP	10	10	m
Number of inhabitants of region	2E+07	4.69E+07	eq
Windspeed in the system	3	3	m/s
<i>Raw sewage</i>			
Mass of O ₂ binding material per person per day	54	49	g/eq/d

Table 1. Continued.

Input items	EU TGD default values	Input values of this study	Unit
Dry weight solids produced per person per day	0.09	0.064	kg/eq/d
Density solids in raw sewage	1.5	1.5	kg/l
Fraction of organic carbon in raw sewage sludge	0.3	0.3	kg/kg
<i>Primary settler</i>			
Depth of primary settler	4	3.6 (3) [#]	m
Hydraulic retention time of primary settler	2	2	hr
Density suspended and settled solids in primary settler	1.5	1.5	kg/l
Fraction of organic carbon in settled sewage sludge	0.3	0.3	kg/kg
<i>Activated sludge tank</i>			
Depth of aeration tank	3	3.3(5) [#]	m
Density solids of activated sludge	1.3	1.3	kg/l
Concentration solids of activated sludge	4	3.6(1.87) [#]	kg/m ³
Steady state O ₂ concentration in activated sludge	2E-03	2E-03	kg/m ³
Mode of aeration	Surface	Surface	-
Fraction of organic carbon in activated sewage sludge	0.37	0.37	kg/kg
Sludge loading rate	0.15	0.304	kg/kg/d
<i>Solids-liquids separator</i>			
Depth of solid-liquid separator	3	3.2	m
Density suspended and settled solids in solid-liquid separator	1.3	1.3	kg/l
Concentration solids in effluent	30	27(24) [#]	mg/l
Hydraulic retention time of solid-liquid separator	6	5.4(3) [#]	hr
Fraction of organic carbon in effluent sewage sludge	0.37	0.37	kg/kg
Regional and continental distribution			
<i>Continental</i>			
Area of EU	3.56E+06	9.94E+04	km ²
Number of inhabitants in the EU	3.7E+08	4.69E+07	eq
Area fraction of water of the continental system	0.03	0.04	-
Area fraction of natural soil	0.6	0.66	-
Area fraction of agricultural soil	0.27	0.25	-
Area fraction of industrial /urban soil	0.1	0.05	-
Fraction of water flow from global scale to continent	0	0	0
Water depth of system	3	4.7	m
Suspended solids concentration of continental system	25	12.7	mg/l
<i>Regional</i>			
Area of regional system	4E+04	9.75E+04	km ²
Number of inhabitants of region	2E+07	4.64E+07	eq
Area fraction of water of the regional system	0.03	0.04	-
Area fraction of natural soil	0.6	0.66	-
Area fraction of agricultural soil	0.27	0.25	-
Area fraction of industrial /urban soil	0.1	0.05	-
Fraction of water flow from continental scale to region	0.034	1	-
Water depth of system	3	4.7	m
Suspended solids concentration of regional system	15	12.7	mg/l
<i>Air</i>			
Atmospheric mixing height	1000	1000	m
Windspeed in the system	3	3	m/s
Aerosol deposition velocity	1E-03	1E-03	m/s
Aerosol collection efficient	2E+05	2E+05	-

Table 1. Continued.

Input items	EU TGD default values	Input values of this study	Unit
Average annual precipitation	700	1274	mm/yr
<i>Water and sediment</i>			
Concentration biota	1	1	mg/l
Sediment mixing depth	0.03	0.03	m
Settling velocity of suspended solids	2.5	2.5	m/d
biogenic production of suspended solids in water	0	0	kg/d
<i>Soil</i>			
Mixing depth natural soil	0.05	0.05	m
Mixing depth agricultural soil	0.2	0.2	m
Mixing depth industrial/urban soil	0.05	0.05	m
Fraction of rain water infiltration soil	0.25	0.25	—
Fraction of rain water running off soil	0.25	0.25	—
Soil erosion rate of regional system	0.03	0.03	mm/yr
<i>Mass transfer</i>			
Air-film PMTC (air-water)	1.39E-03	1.39E-03	m/s
Water-film PMTC (air-water)	1.39E-05	1.39E-05	m/s
Air-film PMTC (air-soil)	1.39E-03	1.39E-03	m/s
Soil-air PMTC (air-soil)	5.56E-06	5.56E-06	m/s
Soil-water film PMTC (air-soil)	5.56E-10	5.56E-10	m/s
Water film PMTC (sediment-water)	2.78E-06	2.78E-06	m/s
Pore water PMTC (sediment-water)	2.78E-08	2.78E-08	m/s
<i>Local distribution</i>			
Air and surface water			
Concentration in air at source strength 1 (kg/d)	2.78E-04	2.78E-04	mg/m ³
Standard deposition flux of aerosol-bound compounds	0.01	0.01	mg/m ² /d
Dilution factor	10	10	—
<i>Soil</i>			
Mixing depth of gaseous soil	0.1	0.1	m
Dry sludge application rate on agricultural soil	5E+03	0	kg/ha/yr
Dry sludge application rate on grassland	1000	0	kg/ha/yr
Averaging time soil (for terrestrial ecosystem)	30	30	d
Averaging time agricultural soil	180	180	d
Averaging time grassland	180	180	d
Air-film PMTC (air-soil)	1.39E-03	1.39E-03	m/s
Soil-air PMTC (air-soil)	5.56E-06	5.56E-06	m/s
Soil-water film PMTC (air-soil)	5.56E-10	5.56E-10	m/s
Mixing depth agricultural soil	0.2	0.2	m
Fraction of rain water infiltration soil	0.25	0.25	—
Average annual precipitation	700	1274	mm/yr
Substance			
<i>Substance identification</i>			
General name	—	Acetanilide	
Description	—		
CAS No.	—	103-84-4	
<i>Physico-chemical properties</i>			
Molecular weight	—	135.17	g/mol
Melting point	—	114.3	°C
Boiling point	—	305	°C

Table 1. Continued.

Input items	EU TGD default values	Input values of this study	Unit
Vapor pressure at 25°C	—	0.1626	Pa
Octanol-water partition coefficient	—	1.16	log10
Water solubility	—	4000	mg/l
Release estimation			
Characterization and tonnage			
High production volume chemical	No	Yes	
Production volume of chemical in Korea	0	2306	ton/yr
Volume of chemical imported to Korea	0	0.95	ton/yr
Volume of chemical exported from Korea	0	15.4	ton/yr
Use patterns			
<i>Emission input data</i>			
Industry category	15/0 others	3 Chemical industry	
Use category	55/0 others	Intermediate	
Fraction of tonnage for application	1	1	—
Fraction of chemical in formulation	1	1	—
Production	Yes	Yes	
Formulation	Yes	Yes	
Processing	Yes	Yes	
Private use	Yes	No	
Recovery	Yes	Yes	
Degradation and transformation rates			
<i>Characterization and STP</i>			
Characterization of biodegradability	Not biodegradable	Rapidly biodegradable	
Degradation calculation method in STP	First order, standard	First order, standard	
Rate constant for degradation in STP	0	24	1/d
Total rate constant for degradation in STP	0	24	1/d
Maximum growth rate of specific microorganisms	2	2	1/d
Half saturation concentrations	0.5	0.5	g/m ³
Effects			
<i>Microorganism</i>			
EC ₅₀ for microorganism in a STP	—	2,589	mg/l
<i>Aquatic organism</i>			
LC ₅₀ for fish	—	10	mg/l
L(E)C ₅₀ for daphnia	—	—	mg/l
EC ₅₀ for algae	—	—	mg/l
NOEC for fish	—	—	mg/l
NOEC for daphnia	—	—	mg/l
NOEC for algae	—	—	mg/l
<i>Terrestrial organism</i>			
LC ₅₀ for plants	—	—	mg/l
LC ₅₀ for earthworms	—	—	mg/l
EC ₅₀ for microorganism	—	—	mg/l
<i>Mammalian</i>			
<i>Acute</i>			
Oral LD ₅₀		1210	mg/kg

Table 1. Continued.

Input items	EU TGD default values	Input values of this study	Unit
Dermal LD ₅₀		1210	mg/kg
Inhalatory LD ₅₀		4030	mg/kg
<i>(Sub)Chronic</i>			
Oral NOAEL		10	mg/kg-d
Oral LOAEL		50	mg/kg-d
Inhalatory NOAEL		33.3	mg/m ³
Inhalatory LOAEL		167	mg/m ³
Dermal NOAEL		10	mg/kg-d
Dermal LOAEL		50	mg/kg-d
NOEC via food		400	mg/kg
Duration of (sub)chronic oral test		chronic	
Species for conversion of NOAEL to NOEC		Canis domestics	
Body weight			
<i>(Sub)Chronic</i>			
Oral NOAEL		0.5	mg/kg-d
Oral LOAEL		2.5	mg/kg-d
Inhalatory NOEC in a medium		1.67	mg/m ³
Inhalatory LOEC in a medium		8.33	mg/m ³
Dermal NOAEL		0.5	mg/kg-d
Dermal LOAEL		2.5	mg/kg-d
<i>Current classification</i>			
Corrosive		No	
Irritating to skin		Yes	
Irritating to eyes		Yes	
Risk of serious damage to eyes		Yes	
Irritation to respiratory system		Yes	
May cause sensitisation by inhalation		Yes	
May cause sensitisation by skin contact		Yes	
May cause cancer		No	
May cause cancer by inhalation		No	
Possible risk of irreversible effects		Yes	

3) Environmental exposure and fate

Acetanilide may be released into the environment at various waste streams from its production and use sites. It is used as intermediates in drug and dye production, as stabilizers in hydrogen peroxide and cellulose esters, as a plasticizer, and as a rubber accelerator, in general.

If released to the atmosphere, acetanilide is expected to exist as a vapor in the ambient atmosphere based on the extrapolated vapor pressure of 1.2×10^{-3} mmHg (0.16 Pa) at 25°C. Acetanilide is not expected to undergo direct photolysis in the environment due

to the lack of functional groups to absorb UV light. It is, however, expected to degrade rapidly by reaction with photochemically-produced hydroxyl radicals (estimated half-life of 30 hours).

If released into the soil, acetanilide is expected to exhibit very high mobility based on a measured K_{oc} of 27 and estimated K_{oc} of 38, using an experimental log K_{ow} of 1.16 and a regression-derived equation. Acetanilide is not expected to volatilize from wet soil based on an estimated Henry's law constant of 6.2×10^{-9} or 5.3×10^{-8} atm-m³/mol and expected to volatilize slightly from dry soil based on an extrapolated

vapor pressure of 1.2×10^{-3} mmHg.³⁾

If released into water, biodegradation of acetanilide is expected to be an important removal process. Several tests indicate that its biodegradation rate under aerobic conditions was >90% after 20 days as BOD and after 5 days as COD.⁴⁾ An estimated bio-concentration factor (BCF) of 4.5 suggests that bio-concentration of acetanilide in aquatic organisms is low (Hansch *et al.*, 1995; Franke *et al.*, 1994).⁵⁾⁻⁶⁾ An earlier reference⁷⁾ also reports that BCF of acetanilide in goldfish *Carassius auratus* is calculated as 1.23, a very low figure. Hydrolysis, adsorption to soil, and volatilization are not expected to be environmentally important removal processes in aquatic systems.

4) Predicted environmental concentration

Acetanilide should be produced and utilized under a well-controlled system on any site, so that the amount of release to environmental compartments is relatively small. The waste of acetanilide from the manufacturing site is released to air and water phases after being treated in its own treatment system.

The potential environmental emission of acetanilide was calculated employing the EUSES system,²⁾ on the basis that regional in the protocol represents the peninsular of South Korea and local is the sewage treatment plant connected to a manufacturing plant located in Ulsan area (Table 1). Environmental data for Taejon area were substituted because of its easy availability. From this, local and regional emissions

Table 2. Local and regional emissions of acetanilide to compartments

Compartment	Local emission (kg/day)	Regional emission (kg/day)	Ratio of emission among compartments in region (%)
Air	19.2	15.8	21.2
Wastewater	80.9	57.0	76.3
Industrial soil	—	1.88	2.5
Surface water*	—	(24.4)	(32.7)
Total	100.1	74.7	100

* Portion of emission disposed from sewage treatment plant to surface water after treatment.

into different compartments are given in Table 2.

This chemical is produced and used in a non-dispersive manner as intermediates of pharmaceuticals and dyes, and is not intrinsically present in consumer products. It is, therefore, assumed that its release to the environment occurs only from the local manufacturing site, through air and wastewater.

The manufacturing system of acetanilide may not be well-controlled in practice and the worst case was, therefore, assumed in calculation of exposures. The distribution of emitted acetanilide at equilibrium in the environmental compartments was obtained for the fugacity level I by means of EQC model and the results are shown in Table 3. It is evident that water system is the major compartment showing the highest distribution.

The predicted environmental concentration (PEC) was obtained through the EUSES system. The results calculated under the first order kinetics and Monod kinetics considering biodegradation for regional scale are given in Table 4 and those for local scale under

Table 3. Estimated equilibrium distribution of acetanilide (Fugacity model, Level I)

Compartment	Distribution (%)
Air	0.11
Water	98.6
Soil	1.26
Sediment	0.03

Table 4. PEC data for regional scale by different kinetics of biodegradation

Compartment	First order kinetics (standard)	Monod kinetics	Unit
Air (total)	1.21×10^{-8}	1.21×10^{-8}	mg/m ³
Surface water (dissolved)	5.47×10^{-5}	9.14×10^{-5}	mg/l
Agricultural soil (total)	1.19×10^{-5}	1.19×10^{-5}	mg/kg wwt
Pore water of agric. soils	3.82×10^{-5}	3.83×10^{-5}	mg/l
Natural soil (total)	2.09×10^{-5}	2.09×10^{-5}	mg/kg wwt
Industrial soil (total)	7.15×10^{-5}	7.15×10^{-5}	mg/kg wwt
Sediment (total)	4.32×10^{-5}	7.23×10^{-5}	mg/kg wwt

Table 5. PEC data for local scale in formulation and processing stages of acetanilide, according to first order kinetics of biodegradation

Compartment	Formulation	Processing	Unit
Air during emission episode	5.31×10^{-3}	1.39×10^{-5}	mg/m ³
Annual average in air, 100 m from point source	4.36×10^{-3}	5.21×10^{-6}	mg/m ³
Surface water during emission episode	9.73×10^{-3}	2.46×10^{-2}	mg/l
Annual average in surface water	7.99×10^{-3}	9.24×10^{-3}	mg/l
Sediment during emission episode	9.99×10^{-3}	2.52×10^{-2}	mg/kg wwt
Agric. soil, over 180 days	7.53×10^{-4}	2.18×10^{-5}	mg/kg wwt
Grassland, over 180 days	1.18×10^{-3}	2.23×10^{-5}	mg/kg wwt
Groundwater under agric. Soil	2.42×10^{-3}	7.00×10^{-5}	mg/kg wwt

the first order kinetics are given in Table 5.

The PEC on a regional scale was in the order of 10^{-8} mg/m³ in air, and in the order of 10^{-5} mg/kg in water and soil/sediment. In a survey conducted in U.S.A., acetanilide was not detected in river water⁸⁾ and sediment.

As any of the local monitoring data in Korea is not available, PEC in surface water during emission episode for local scale was calculated using the EUSES system to be 0.02 mg/l, as the worst case. The concentration of acetanilide in wastewater from a plant in U.S.A. was analysed to be 0.2 mg/l and not detected in sediment.⁸⁾ It appears that there is a significant difference between the predicted wastewater concentration and the figure from the monitoring data.

3. Ecotoxicity

Ecotoxicological data exist on acute toxicity to fishes of 4 species only. No data are available on acute toxicities of other organisms or chronic toxicity to fishes. LC₅₀ value for bluegill sunfish and paddy fish (100 mg/l) was used to calculate the PNEC according to the EUSES system. Assessment factor to derive the PNEC for the water compartment was 1,000, since short-term toxicity data were available

only for fishes. The result is given in Table 5 and the lowest PNEC value of 0.1 mg/l, derived from 2 species of fish, was used for the calculation of RCR for acetanilide. No experimental data are available on the effects on terrestrial organisms and it was not attempted to calculate PNEC values.

4. Initial ecological risk assessment

Predicted no effect concentration (PNEC) of acetanilide has been calculated as 0.1 mg/l for aquatic organism (fish). Predicted environmental concentration (PEC) in the surface water on a regional scale was estimated to be 9.1×10^{-5} mg/l as the worst case. Thus, risk characterisation ratio (RCR) of acetanilide for aquatic organism is simply calculated as follows :

$$\begin{aligned} \text{RCR}_{\text{fish, regional}} &= \text{PEC}/\text{PNEC} \\ &= 9.1 \times 10^{-5}/0.1 = 9.1 \times 10^{-4} \ll 1 \end{aligned}$$

If RCR is below 1, the chemical is considered of low priority for further work, whereas RCR is equal or above 1, the chemical is considered for further

Table 6. Predicted no effect concentration (PNEC) of acetanilide toward fish

Species	Exposure	LC ₅₀ (mg/l)	PNEC (mg/l)
<i>Leuciscos idus</i> (Ide)	Acute (48 hr)	200	0.2
<i>Lepomis macrochirus</i> (Bluegill sunfish)	Acute (96 hr)	100	0.1
<i>Menidia beryllina</i> (Inland silverside)	Acute (96 hr)	115	0.1
<i>Oryzias latipes</i> (Paddy fish)	Acute (96 hr)	> 100	> 0.1

Table 7. RCR of acetanilide in local and regional environments as estimated by EUSES system*

Environmental compartment	Local exposure		Regional exposure
	Formulation	Processing	
Water	0.13	0.25	9.14×10^{-4}
Soil	0.02	7.0×10^{-4}	3.83×10^{-4}
Sediment	0.16	0.31	8.75×10^{-4}
Sewage treatment plant	4.80×10^{-3}	9.51×10^{-3}	—
Birds & mammals	2.51×10^{-4}	2.26×10^{-4}	—

* Input data into EUSES model: LC₅₀ for fish : 100 mg/l
EC₅₀ for microorganisms in STP : 2,589 mg/l
Oral LD₅₀ for mammals (mouse, acute) : 1,210 mg/kg

work, according to OECD context.

It is evident that acetanilide will not cause any adverse effect toward aquatic organisms on a regional scale since all of RCR values are below 0.001, equivalent to safety margin of 1,000. RCR calculated for different environmental compartments employing the EUSES system is given in Table 6. The higher value in RCR was adopted among data from first order and Monod kinetics in regard to biodegradation.

RCR is far below 1 in general when the toxicity data on fish only is applied. At present, it is considered that acetanilide may not exhibit any adverse effect in aquatic organisms on a regional basis. However, RCR on a local basis approaches 0.2 in water and sediment which may not bring about any adverse effects on the aquatic organisms according to the OECD context. However, additional data on the acute toxicity to daphnia or toxicity to algae may be needed for refined risk assessment of acetanilide.

ABSTRACT

Acetanilide may be released into the environment through air and wastewater from its production and use sites as an intermediate in the synthesis of pharmaceuticals and dyes. Acetanilide is biodegraded rapidly under aerobic conditions and decomposed by indirect photolysis in the presence of OH radicals. An estimated bioconcentration factor of 4.5 suggests that bioaccumulation in aquatic organisms is low.

Ecotoxicological data on acetanilide exist on acute toxicity to fishes of 4 species only. According to the EUSES system, the lowest PNEC (Predicted no effect concentration) in fishes is 0.01 mg/l and PEC (Predicted environmental concentration) for surface water on a regional scale is 9.1×10^{-5} mg/l as the worst case. RCR (Risk characterization ratio) of acetanilide for surface water on a regional scale was estimated as 9.1×10^{-3} , which is safe enough for fi-

shes. RCR on a local basis slightly exceeds the value 1 in water and sediment; that is, 1.3 and 1.6, respectively, which suggests the existence of ecotoxicological risk at the vicinity of the manufacturing site.

For the refinement of environmental risk assessment on acetanilide, more data should be collected regarding prolonged fish toxicity, acute toxicity toward daphnia and algae. It is, therefore, recommended that acetanilide should be a candidate for further work to supplement the lacking data until it is proved to be safe in the ecotoxicological aspects.

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