

**Index of Revised Robust Summaries
FND Cationics HPV Chemicals Challenge**

June 26, 2003

Supplement to
Appendix A

**Index of Revised Robust Summaries
for ACC FND HPV Cationics Task Force**

Page

3.3.2 TRANSPORTATION BETWEEN ENVIRONMENTAL COMPARTMENTS (FUGACITY MODEL)

1. Ammonium, dodecyltrimethyl-, chloride (CAS RN 112-00-5) Mackay, Level III Fugacity Model.	1
2. Ammonium, hexadecyltrimethyl-, chloride (CAS RN 112-02-7) Mackay, Level III Fugacity Model.	3
3. Trimethyloctadecylammonium chloride (CAS RN 112-03-8) Mackay, Level III Fugacity Model.	5
4. 1-Hexadecanaminium, N, N-dihexadecyl-N-methyl-, chloride (CAS RN 52467-63-7; Tricetylmethyl ammonium chloride, TMAC) Mackay, Level III Fugacity Model.	7
5. Didecyldimethylammonium chloride (CAS RN 7173-51-5) Mackay, Level III Fugacity Model.	9

4.1 ACUTE/PROLONGED TOXICITY TO FISH

6. Ammonium, hexadecyltrimethyl-chloride (CAS RN 112-02-7). Wildish, D. J. and W. G. Carson. 1972. Acute Lethality of Some Nonionic and Cationic Surfactants to <i>S. salar</i> and <i>G. oceanicus</i> . Fisheries Research Board of Canada, Manuscript Report Series number 1212.	11
7. Arquad 3.16 (CAS RN 52467-63-7; Tricetylmethyl ammonium chloride). Jenkins, C. A. 1990. Arquad 3.16: acute toxicity to rainbow trout. Report number 90/AKL011/0347. Life Science Research Limited, Suffolk, UK.	12
8. Arquad 2HT-75 (CAS RN 61789-80-8; Dimethyl di (hydrogenated tallow) ammonium chloride). Dean, W. P. 1977. The Acute Toxicity of Arquad 2HT-75, Dimethyl di (hydrogenated tallow) ammonium chloride 75% active, 1633602, to the Bluegill Sunfish <i>Lepomis machrochirus</i> Rafinesque and Rainbow Trout <i>Salmo gairdneri</i> Richardson. Study number 398-001. International Research and Development Corporation [bluegill]	15
9. Arquad 2HT-75 (CAS RN 61789-80-8; Dimethyl di (hydrogenated tallow) ammonium chloride). Dean, W. P. 1977. The Acute Toxicity of Arquad 2HT-75, Dimethyl di (hydrogenated tallow) ammonium chloride 75% active, 1633602, to the Bluegill Sunfish <i>Lepomis machrochirus</i> Rafinesque and Rainbow Trout <i>Salmo gairdneri</i> Richardson. Study number 398-001. International Research and Development Corporation [trout]	17
10. Arquad 2HT-75 (CAS RN 61789-80-8; Ditalowdimethylammoniumchloride, hydrogenated). Dommröse, A. M. 1987. Investigation of the Lethal Effects of the Test Sample Arquad 2 HT-75 to the Rainbow Trout (OECD 203). NATEC Institute, Hamburg, Germany.	19

**Index of Revised Robust Summaries
for ACC FND HPV Cationics Task Force
(continued)**

	Page
11. Ditallow dimethyl ammonium chloride (DTDMAC; CAS RN 68783-78-8). Lewis, M. A. and V. T. Wee. 1983. Aquatic Safety Assessment for Cationic Surfactants. Microbiological Associates, Bethesda, MD, USA. Unpublished report (No. T1806.501) [bluegill].....	21
12. Ditallow dimethyl ammonium chloride (DTDMAC; CAS RN 68783-78-8). Lewis, M. A. and V. T. Wee. 1983. Aquatic Safety Assessment for Cationic Surfactants. Microbiological Associates, Bethesda, MD, USA. Unpublished report (No. T1806.501) [sheepshead minnow].....	23
 4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES	
13. Dodecyl trimethyl ammonium chloride (C ₁₂ TMAC; CAS RN 112-00-5). Taylor, M. J. 1984. Comparative Sensitivity of <i>Ceriodaphnia Sp.</i> and <i>Daphnia Magna</i> to Select Surfactants. Procter & Gamble Co., Cincinnati, OH, US. Unpublished report (Notebook: ZE-1154 and ME-1082).....	25
14. Monotallowtrimethyl ammonium chloride (CAS RN 8030-78-2; quaternary ammonium compounds, trimethyltallow alkyl, chlorides). Valentine, L. C. and W. E. Bishop. 1992. Effects of MTTMAC on the Survival and Reproduction of <i>Daphnia Magna</i> in Laboratory Waters and a Natural Surface Water. Procter & Gamble Co., Cincinnati, OH, USA. Unpublished report (Notebook: ME- 5004, ME-5007 and ZE-1111) [river water].....	27
15. Monotallowtrimethyl ammonium chloride (CAS RN 8030-78-2; quaternary ammonium compounds, trimethyltallow alkyl, chlorides). Valentine, L. C. and W. E. Bishop. 1992. Effects of MTTMAC on the Survival and Reproduction of <i>Daphnia Magna</i> in Laboratory Waters and a Natural Surface Water. Procter & Gamble Co., Cincinnati, OH, USA. Unpublished report (Notebook: ME- 5004, ME-5007 and ZE-1111) [laboratory blended water]	30
16. Monotallowtrimethyl ammonium chloride (CAS RN 8030-78-2; quaternary ammonium compounds, trimethyltallow alkyl, chlorides). Valentine, L. C. and W. E. Bishop. 1992. Effects of MTTMAC on the Survival and Reproduction of <i>Daphnia Magna</i> in Laboratory Waters and a Natural Surface Water. Procter & Gamble Co., Cincinnati, OH, USA. Unpublished report (Notebook: ME- 5004, ME-5007 and ZE-1111) [Southwest well water]	33
17. Arquad 3.16 (CAS RN 52467-63-7; Tricetylmethyl ammonium chloride). Jenkins, C. A. 1990. Arquad 3.16: acute toxicity to <i>Daphnia magna</i> . Report number 90/AKL012/0348. Life Science Research Limited, Suffolk, UK.....	36

**Index of Revised Robust Summaries
for ACC FND HPV Cationics Task Force
(continued)**

	Page
18. Ditallow dimethyl ammonium chloride (DTDMAC; CAS RN 68783-78-8). Lewis, M. A. and V. T. Wee. 1983. Aquatic Safety Assessment for Cationic Surfactants. Microbiological Associates, Bethesda, MD, USA. Unpublished report (No. T1806.501).	39
 4.3 TOXICITY TO AQUATIC PLANTS (ALGAE)	
19. Arquad 3.16 (CAS RN 52467-63-7; Tricetylmethyl ammonium chloride). Kroon, A. G. M. and Geurts, M. G. J. 1994. Toxicity of Arquad 3.16 to the freshwater alga <i>Selenastrum capricornutum</i> . Report no. CRL F94024, T 93-10-03. Akzo Research Laboratories Arnhem, The Netherlands.	42
20. Ditallow dimethyl ammonium chloride (DTDMAC; CAS RN 68783-78-8). Lewis, M. A. and V. T. Wee. 1983. Aquatic Safety Assessment for Cationic Surfactants. Microbiological Associates, Bethesda, MD, USA. Unpublished report (No. T1806.501).	44
21. Ditallow dimethyl ammonium chloride (DTDMAC; CAS RN 68783-78-8). Shorter, S. J. 1993. The Chronic Effects of DTDMAC on the Fathead Minnow (<i>Pimephales promelas</i>) Larval Survival and Growth. Procter & Gamble Co., Cincinnati, OH, USA. Unpublished report (Report No. E89-006).	46
 4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES	
22. Monotallowtrimethyl ammonium chloride (CAS RN 8030-78-2; quaternary ammonium compounds, trimethyltallow alkyl, chlorides). Valentine, L. C. and W. E. Bishop. 1992. Effects of MTTMAC on the Survival and Reproduction of <i>Daphnia Magna</i> in Laboratory Waters and a Natural Surface Water. Procter & Gamble Co., Cincinnati, OH, USA. Unpublished report (Notebook: ME- 5004, ME-5007 and ZE-1111) [river water]	48
23. Monotallowtrimethyl ammonium chloride (CAS RN 8030-78-2; quaternary ammonium compounds, trimethyltallow alkyl, chlorides). Valentine, L. C. and W. E. Bishop. 1992. Effects of MTTMAC on the Survival and Reproduction of <i>Daphnia Magna</i> in Laboratory Waters and a Natural Surface Water. Procter & Gamble Co., Cincinnati, OH, USA. Unpublished report (Notebook: ME- 5004, ME-5007 and ZE-1111) [Southwest well water]	51

3.3.2 TRANSPORTATION BETWEEN ENVIRONMENTAL COMPARTMENTS (FUGACITY MODEL)

Test Substance

Identity: Ammonium, dodecyltrimethyl-, chloride
 (CAS RN 112-00-5)
 Purity: NA
 Remarks:

Method

Method/Guideline followed: Calculation according to Mackay, Level III
 Media: Water, air, soil and sediment (model run with emissions to water = 1000 kg/hr)
 GLP: NA
 Year: 2003
 Remarks: The EPIWIN model was run using the following physical chemical properties: melting point = 182°C; vapor pressure = 9.27×10^{-9} mm Hg; *n*-octanol/water partition coefficient (Log K_{ow}) = 1.22 and aqueous solubility = 1795 mg/L. Surface water was set as the sole input vector, using the chemical specific parameters to attain estimates of the chemical distributions between environmental compartments.

Results

Remarks: Following are results from the model:

Level III Fugacity Model (Full-Output):

=====

Chem Name : Dodecyltrimethylammonium chloride
 Molecular Wt: 263.9
 Henry's LC : 9.42e-011 atm-m3/mole (Henrywin program)
 Vapor Press : 9.27e-009 mm Hg (Mpbpwin program)
 Liquid VP : 3.32e-007 mm Hg (super-cooled)
 Melting Pt : 182 deg C (Mpbpwin program)
 Log Kow : 1.22 (Kowwin program)
 Soil Koc : 6.8 (calc by model)

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	3.7e-009	9	0
Water	99.8	360	1000
Soil	3.5e-005	360	0
Sediment	0.19	1.44e+003	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	1.17e-020	9.76e-007	1.27e-007	9.76e-008	1.27e-008
Water	6.1e-016	658	342	65.8	34.2
Soil	5.13e-021	0.000231	0	2.31e-005	0
Sediment	4.99e-016	0.313	0.013	0.0313	0.0013

Persistence Time: 342 hr
Reaction Time: 520 hr
Advection Time: 1e+003 hr
Percent Reacted: 65.8
Percent Advected: 34.2

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):

Air: 9.002
Water: 360
Soil: 360
Sediment: 1440
Biowin estimate: 2.914 (weeks)

Advection Times (hr):

Air: 100
Water: 1000
Sediment: 5e+004

Conclusions:

Mass Amounts:

Air = < 0.1%
Water = 99.8%
Soil = 60%
Sediment = 0.2%

Remarks:

The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Cationics Task Group).

Data Quality

Reliability:

2

Remarks:

Reliable with restrictions; model data.

References

Mackay, D., A. DiGuardo, S. Paterson and C.E. Cowan. 1996. Evaluating the Environmental Fate of Variety of Types of Chemicals Using the EQC Model. *Environ. Toxicol. Chem.* 15(9):1627-1637.

Other Available Reports

Other

Last changed:

June 26, 2003

Order number for sorting:

NA

Remarks:

3.3.2 TRANSPORTATION BETWEEN ENVIRONMENTAL COMPARTMENTS (FUGACITY MODEL)

Test Substance

Identity: Ammonium, hexadecyltrimethyl-, chloride
 (CAS RN 112-02-7)
 Purity: NA
 Remarks:

Method

Method/Guideline followed: Calculation according to Mackay, Level III
 Media: Water, air, soil and sediment (model run with emissions to water = 1000 kg/hr)
 GLP: NA
 Year: 2003
 Remarks: The EPIWIN model was run using the following physical chemical properties: melting point = 213°C; vapor pressure = 2.8×10^{-10} mm Hg; *n*-octanol/water partition coefficient (Log K_{ow}) = 3.23 and aqueous solubility = 16.3 mg/L. Surface water was set as the sole input vector, using the chemical specific parameters to attain estimates of the chemical distributions between environmental compartments.

Results

Remarks: Following are results from the model:

Level III Fugacity Model (Full-Output):

=====

Chem Name : Cetrimonium chloride
 Molecular Wt: 320.01
 Henry's LC : 2.93e-010 atm-m3/mole (Henrywin program)
 Vapor Press : 2.8e-010 mm Hg (Mpbpwin program)
 Liquid VP : 2e-008 mm Hg (super-cooled)
 Melting Pt : 213 deg C (Mpbpwin program)
 Log Kow : 3.23 (Kowwin program)
 Soil Koc : 696 (calc by model)

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	3.52e-008	7.51	0
Water	98.5	360	1000
Soil	0.000135	360	0
Sediment	1.52	1.44e+003	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	9.23e-020	1.12e-005	1.22e-006	1.12e-006	1.22e-007
Water	1.56e-015	656	341	65.6	34.1
Soil	1.4e-021	0.000901	0	9.01e-005	0
Sediment	6.8e-016	2.53	0.105	0.253	0.0105

Persistence Time: 346 hr
Reaction Time: 525 hr
Advection Time: 1.02e+003 hr
Percent Reacted: 65.9
Percent Advected: 34.1

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):

Air: 7.514
Water: 360
Soil: 360
Sediment: 1440
Biowin estimate: 2.790 (weeks)

Advection Times (hr):

Air: 100
Water: 1000
Sediment: 5e+004

Conclusions:

Mass Amounts:

Air = < 0.1%
Water = 98.5%
Soil = < 0.1%
Sediment = 1.5%

Remarks:

The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Cationics Task Group).

Data Quality

Reliability:

2

Remarks:

Reliable with restrictions; model data.

References

Mackay, D., A. DiGuardo, S. Paterson and C.E. Cowan. 1996. Evaluating the Environmental Fate of Variety of Types of Chemicals Using the EQC Model. *Environ. Toxicol. Chem.* 15(9):1627-1637.

Other Available Reports

Other

Last changed:

June 26, 2003

Order number for sorting:

NA

Remarks:

3.3.2 TRANSPORTATION BETWEEN ENVIRONMENTAL COMPARTMENTS (FUGACITY MODEL)

Test Substance

Identity: Trimethyloctadecylammonium chloride
 (CAS RN 112-03-8)
 Purity: NA
 Remarks:

Method

Method/Guideline followed: Calculation according to Mackay, Level III
 Media: Water, air, soil and sediment (model run with emissions to water = 1000 kg/hr)
 GLP: NA
 Year: 2003
 Remarks: The EPIWIN model was run using the following physical chemical properties: melting point = 223°C; vapor pressure = 5.35×10^{-11} mm Hg; *n*-octanol/water partition coefficient (Log K_{ow}) = 4.17 and aqueous solubility = 1.759 mg/L. Surface water was set as the sole input vector, using the chemical specific parameters to attain estimates of the chemical distributions between environmental compartments.

Results

Remarks: Following are results from the model:

Level III Fugacity Model (Full-Output):

=====

```
Chem Name   : Octadecyltrimethylammonium chloride
Molecular Wt: 348.06
Henry's LC  : 5.16e-010 atm-m3/mole (Henrywin program)
Vapor Press : 5.35e-011 mm Hg (Mpbpwin program)
Liquid VP   : 4.9e-009 mm Hg (super-cooled)
Melting Pt  : 223 deg C (Mpbpwin program)
Log Kow     : 4.17 (Kowwin program)
Soil Koc    : 6.06e+003 (calc by model)
```

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	9.17e-008	6.94	0
Water	83.3	900	1000
Soil	0.000496	900	0
Sediment	16.7	3.6e+003	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	4.17e-019	6.06e-005	6.07e-006	6.06e-006	6.07e-007
Water	4.05e-015	425	552	42.5	55.2
Soil	1.86e-021	0.00253	0	0.000253	0
Sediment	2.8e-015	21.3	2.21	2.13	0.221

Persistence Time: 662 hr
Reaction Time: 1.48e+003 hr
Advection Time: 1.2e+003 hr
Percent Reacted: 44.6
Percent Advected: 55.4

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):

Air: 6.941
Water: 900
Soil: 900
Sediment: 3600
Biowin estimate: 2.728 (weeks-months)

Advection Times (hr):

Air: 100
Water: 1000
Sediment: 5e+004

Conclusions:

Mass Amounts:

Air = < 0.1%
Water = 83.3%
Soil = < 0.1%
Sediment = 16.7%

Remarks:

The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Cationics Task Group).

Data Quality

Reliability:

2

Remarks:

Reliable with restrictions; model data.

References

Mackay, D., A. DiGuardo, S. Paterson and C.E. Cowan. 1996. Evaluating the Environmental Fate of Variety of Types of Chemicals Using the EQC Model. *Environ. Toxicol. Chem.* 15(9):1627-1637.

Other Available Reports

Other

Last changed:

June 26, 2003

Order number for sorting:

NA

Remarks:

3.3.2 TRANSPORTATION BETWEEN ENVIRONMENTAL COMPARTMENTS (FUGACITY MODEL)

Test Substance

Identity: 1-Hexadecanaminium, N, N-dihexadecyl-N-methyl-, chloride
 (CAS RN 52467-63-7; Tricetylmethyl ammonium chloride, TMAC)
 Purity: NA
 Remarks:

Method

Method/Guideline followed: Calculation according to Mackay, Level III
 Media: Water, air, soil and sediment (model run with emissions to water = 1000 kg/hr)
 GLP: NA
 Year: 2003
 Remarks: The EPIWIN model was run using the following physical chemical properties: melting point = 46°C; vapor pressure = 1.8 mm Hg; *n*-octanol/water partition coefficient (Log K_{ow}) = 5.9 and aqueous solubility = 10 mg/L (O'Connor, 1990). Surface water was set as the sole input vector, using the chemical specific parameters to attain estimates of the chemical distributions between environmental compartments.

Results

Remarks: Following are results from the model:

Level III Fugacity Model (Full-Output):

```

=====
Chem Name      : TRICETYLMETHYLAMMONIUM CHLORIDE
Molecular Wt  : 740.82
Henry's LC    : 0.175 atm-m3/mole (calc VP/Wsol)
Vapor Press   : 1.8 mm Hg (user-entered)
Liquid VP     : 2.9 mm Hg (super-cooled)
Melting Pt    : 46 deg C (user-entered)
Log Kow       : 5.9 (user-entered)
Soil Koc      : 3.26e+005 (calc by model)
    
```

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	0.0799	2.78	0
Water	12.7	900	1000
Soil	0.00166	900	0
Sediment	87.2	3.6e+003	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	4.27e-013	323	12.9	32.3	1.29
Water	1.59e-007	158	206	15.8	20.6
Soil	4.54e-014	0.0208	0	0.00208	0
Sediment	1.07e-007	272	28.3	27.2	2.83

Persistence Time: 1.62e+003 hr
Reaction Time: 2.15e+003 hr
Advection Time: 6.57e+003 hr
Percent Reacted: 75.3
Percent Advected: 24.7

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):

Air: 2.779
Water: 900
Soil: 900
Sediment: 3600
Biowin estimate: 2.457 (weeks-months)

Advection Times (hr):

Air: 100
Water: 1000
Sediment: 5e+004

Conclusions:

Mass Amounts:

Air = < 0.1%
Water = 12.7%
Soil = < 0.1%
Sediment = 87.2%

Remarks:

The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Cationics Task Group).

Data Quality

Reliability:

2

Remarks:

Reliable with restrictions; model data.

References

Mackay, D., A. DiGuardo, S. Paterson and C.E. Cowan. 1996. Evaluating the Environmental Fate of Variety of Types of Chemicals Using the EQC Model. *Environ. Toxicol. Chem.* 15(9):1627-1637.

Other Available Reports

O'Connor, J. 1990. Arquad 3.16: Determination of Physico-Chemical Properties. Report number 90/AKL013/0587. Akzo Chemicals International, BV, The Netherlands

Other

Last changed:

June 26, 2003

Order number for sorting:

NA

Remarks:

3.3.2 TRANSPORTATION BETWEEN ENVIRONMENTAL COMPARTMENTS (FUGACITY MODEL)

Test Substance

Identity: Didecyl-dimethylammonium chloride (DDAC)
 (CAS RN 7173-51-5)
 Purity: NA
 Remarks:

Method

Method/Guideline followed: Calculation according to Mackay, Level III
 Media: Water, air, soil and sediment (model run with emissions to water = 1000 kg/hr)
 GLP: NA
 Year: 2003
 Remarks: The EPIWIN model was run using the following physical chemical properties: melting point = 229°C; vapor pressure = 2.33×10^{-11} mm Hg; *n*-octanol/water partition coefficient (Log K_{ow}) = 0.00 and aqueous solubility = 700 mg/L. Surface water was set as the sole input vector, using the chemical specific parameters to attain estimates of the chemical distributions between environmental compartments.

Results

Remarks: Following are results from the model:

Level III Fugacity Model (Full-Output):

=====

Chem Name : Didecyl-dimethylammonium chloride (Bardac 22)
 Molecular Wt: 362.09
 Henry's LC : 6.85e-010 atm-m3/mole (Henrywin program)
 Vapor Press : 2.33e-011 mm Hg (Mpbpwin program)
 Liquid VP : 2.42e-009 mm Hg (super-cooled)
 Melting Pt : 229 deg C (Mpbpwin program)
 Log Kow : 0 (user-entered)
 Soil Koc : 0.41 (calc by model)

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	1.95e-007	5.54	0
Water	99.8	360	1000
Soil	0.000222	360	0
Sediment	0.168	1.44e+003	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	4.36e-019	8.35e-005	6.68e-006	8.35e-006	6.68e-007
Water	3.23e-015	658	342	65.8	34.2
Soil	2.58e-019	0.00146	0	0.000146	0
Sediment	2.69e-015	0.276	0.0115	0.0276	0.00115

Persistence Time: 342 hr
Reaction Time: 520 hr
Advection Time: 1e+003 hr
Percent Reacted: 65.8
Percent Advected: 34.2

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):

Air: 5.544
Water: 360
Soil: 360
Sediment: 1440
Biowin estimate: 2.996 (weeks)

Advection Times (hr):

Air: 100
Water: 1000
Sediment: 5e+004

Conclusions:

Mass Results:

Air = < 0.1%
Water = 99.8%
Soil = < 0.1%
Sediment = 0.2%

Remarks:

The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Cationics Task Group).

Data Quality

Reliability:

2

Remarks:

Reliable with restrictions; model data.

References

Mackay, D., A. DiGuardo, S. Paterson and C.E. Cowan. 1996. Evaluating the Environmental Fate of Variety of Types of Chemicals Using the EQC Model. *Environ. Toxicol. Chem.* 15(9):1627-1637.

Other Available Reports

Other

Last changed:

June 26, 2003

Order number for sorting:

NA

Remarks:

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Test Substance

Identity: Ammonium, hexadecyltrimethyl-chloride
(CAS RN 112-02-7)
Purity: 50%
Remarks:

Method

Method/guideline followed: Non-specific test method.
Type: Static acute
GLP: No
Year: 1972
Species/Strain/Supplier: Atlantic salmon *Salmo salar*/NA/St. John Fish Culture Station
Analytical Monitoring: No
Exposure Period: 24 hours
Statistical Methods: Not stated
Remarks: Fish used in testing ranged from 8.2 to 11.7 cm in length and weighed 5.1 to 14.1 g. Concentrations used in testing were corrected for active ingredient content.

Results

Nominal concentrations (mg/l): Not stated
Measured concentrations (mg/l): Not stated
Unit: mg/l
Element Value: 24-hour LC₅₀ = 0.07 mg/l
Statistical Results: 24-hour LC₅₀ = 0.07 mg/l
Result: 24-hour LC₅₀ = 0.07 mg/l
Remarks:

Conclusions

The 24-hour acute toxicity of the test substance to *Salmo salar* was adequately characterized by the study.

Data Quality

Reliability (Klimisch): 2B
Remarks: Reliable with restrictions; basic data given, comparable to guidelines/standards.

References

Wildish, D. J. and W. G. Carson. 1972. Acute Lethality of Some Nonionic and Cationic Surfactants to *S. salar* and *G. oceanicus*. Fisheries Research Board of Canada, Manuscript Report Series number 1212.

Other Available Reports

Other

Last Changed: September 4, 2003 lam
Order number for sorting: 4a
Remarks:

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Test Substance

Identity: Arquad 3.16 (CAS RN 52467-63-7;
Tricetylmethyl ammonium chloride)
Purity: 86.0 %
Remarks:

Method

Method/Guideline followed: OECD Guidelines for Testing of Chemicals, Fish, Acute Toxicity Test, Procedure 203, adopted 4 April 1984
Type: Semistatic
GLP: Yes
Year: 1990
Species/Strain/Supplier: Rainbow trout supplied by Hauxton Fisheries Services, Cambridge
Analytical monitoring: Yes
Exposure period: 96 hours
Statistical methods: Median lethal concentrations calculated using the computer program of Stephan; because measured concentrations were not all within 20% of their respective nominal values. LC₅₀ values were calculated using means of measured concentrations.
Remarks: Based on the results of a range-finding study, groups of ten juvenile rainbow trout/group were exposed to the test substance at nominal concentrations of 2.5, 5.0, 10.0, 20.0, 40.0 and 80.0 mg/l for 96 hours under static conditions. A control group was treated with dilution water alone. Fish were transferred to vessels containing freshly prepared test or control media at 48 hours. The mean wet weight of the fish, based on a sample of ten fish taken at random from the holding tank was 1.0 g. The mean fork length of these fish was 4.25 cm. The dilution water was treated tap water. Test dilutions were prepared individually from an aqueous stock dispersion (nominally 1000 mg/l), which had been treated by ultrasound for 30 minutes. The test vessels were all-glass aquaria with a total capacity of 15 liters. Aeration of the contents of each vessel was achieved using a Pasteur pipette connected to an oil-free supply of compressed air. All glassware was conditioned to the test substance for approximately 48 hours before use. Observations of fish were made frequently during the initial four hours of test and thereafter at 24-hour intervals. Concentrations of the test substance were measured in mid-vessel samples at each exposure concentration during the test.

Results

Nominal concentrations (mg/l):	2.5, 5.0, 10.0, 20.0, 40.0 and 80.0 mg/l
Measured concentrations (mg/l):	2.29, 7.72, 12.5, 20.1, 59.4 and 110.8 mg/l (by HPLC)
Unit:	mg/l
Elemental Value:	24-hour LC ₅₀ = 19.2
(as measured concentrations)	(95% Confidence Interval, CI = 13.8 and 26.9 mg/l)
	48-hour LC ₅₀ ~ 15.1
	72-hour LC ₅₀ ~ 15.1
	96-hour LC ₅₀ ~ 14.5
Statistical results:	Described above
Remarks:	The highest nominal concentration at which no mortality occurred and lowest at which there was 100% mortality after 96 hours were 5.0 and 20.0 mg/l, respectively. Mortality was not progressive during the test; the majority of the deaths occurred within the first 24 hours. No adverse effects were observed in test dilutions containing the test substance at nominal concentrations of 2.5 and 5.0 mg/l. The no observed effect concentration was considered to be 5.0 mg/l. Cumulative mortalities were as follows:

Dose level (mg/l)	Minutes	Hours					
	15	2	4	24	48	72	96
0	0/10	0/10	0/10	0/10	0/10	0/10	0/10
2.5	0/10	0/10	0/10	0/10	0/10	0/10	0/10
5.0	0/10	0/10	0/10	0/10	0/10	0/10	0/10
10.0	0/10	0/10	0/10	1/10	1/10	1/10	2/10
20.0	0/10	0/10	0/10	8/10	10/10	10/10	10/10
40.0	0/10	1/10	7/10	10/10	10/10	10/10	10/10
80.0	0/10	9/10	10/10	10/10	10/10	10/10	10/10

At all concentrations, test preparations were white, hazy dispersions with particulate material present on their surfaces. At 40 and 80 mg/l, the opacity of the media made it difficult to observe the fish at the start of the test. The appearance of these test dilutions did not change during the test.

Water quality measurements taken before and during the test ranged as follows: temperatures of 13.1 to 14.3°C; pH of 7.72 to 8.42; percent dissolved oxygen of 90 to 101%; and total hardness of 206 to 220 mg/l as CaCO₃.

Conclusions

Remarks: The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Cationics Task Group).

Data Quality

Reliability (Klimisch): 1A

Remarks: Reliable without restriction; Guideline study.

References

Jenkins, C. A. 1990. Arquad 3.16: acute toxicity to rainbow trout. Report number 90/AKL011/0347. Life Science Research Limited, Suffolk, UK.

Other Available Reports

Other

Last changed: May 14, 2003

Order number for sorting: 33

Remarks:

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Test Substance

Identity: Arquad 2HT-75 (CAS RN 61789-80-8;
Dimethyldi (hydrogenated tallow) ammonium chloride)
Purity: 75%
Remarks:

Method

Method/guideline followed: Test procedures followed EPA 1975, Methods for acute toxicity tests with fish, macroinvertebrates and amphibians (EPA 660/3-75-00)

Type: Static acute

GLP: No

Year: 1977

Species/Strain/Supplier: Bluegill *Lepomis macrochirus*/NA/commercial supplier

Analytical Monitoring: No

Exposure Period: 96 hours

Statistical Methods: Spearman-Kärber LC₅₀ calculations (Finney 1971)

Remarks: The study measured the acute toxicity of the test substance to bluegill during a 96-hour static exposure period. Fish were maintained in the laboratory until testing. Water used for holding and testing was reconstituted soft deionized well water having approximately the following: pH 7.6, total hardness 43 mg/l as CaCO₃, total alkalinity 28 mg/l as CaCO₃, and specific conductance 180 ? mhos/cm. Bluegill at the time of testing were approximately 7 months old and had a mean length of 40 mm and a mean weight of 0.97 g. Forty-eight hours prior to the test, feeding was ceased. Five exposure levels and a control were used in the test. No replication of test levels was used. Test substance was melted in a hot-water bath, weighed and diluted to volume in volumetric glassware with deionized water. Test vessels were 5-gallon glass containers holding 15 liters of test solution. Tests were initiated by introducing the test substance into the vessels containing dilution water, thoroughly mixing the solutions, then introducing the fish. Ten fish were placed into each test vessel. Fish loading in the test was 0.65 g/l. Observations for deaths and abnormal behavioral effects were made at 24, 48 and 96 hours. Dissolved oxygen and pH were measured regularly through study for the control, low, medium, and high test concentration levels.

Results

Nominal concentrations (mg/l): 0 (control), 0.56, 1.0, 1.8, 3.2, and 5.6 mg/l
Measured concentrations (mg/l): N/A

Unit: mg/l
Element Value: LC₅₀ (95% confidence interval)
Statistical Results: 96-hour LC₅₀ = 1.33 mg/l (1.07 – 1.65 mg/l)
Result: Additional results included the following:
48-hour LC₅₀ = 1.33 mg/l (1.07 – 1.65)
24-hour LC₅₀ = 2.36 mg/l (*95% confidence interval could not be calculated due to lack of partial kills*)

96-hour NOEC = 0.56 mg/l
Remarks: 100% mortality occurred in the 3.2 and 5.6 mg/l treatments, while 80% and 20% mortality occurred at 1.8 and 1.0 mg/l, respectively. No mortality occurred at 0.56 mg/l. Behavioral observations made during the test indicated that bluegill exposed to 1.0 mg/l and higher became disoriented, demonstrated erratic swimming behavior and showed signs of varied discoloration. Temperature averaged 22.0 ± 1°C, and the dissolved oxygen concentration and pH during the study ranged from 5.0 to 8.8 mg/l and from 7.07 to 7.58, respectively.

Conclusions

The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Cationics Task Group).

Data Quality

Reliability (Klimisch): 1B
Remarks: Reliable without restriction; comparable to guideline study

References

Dean, W. P. 1977. The Acute Toxicity of Arquad 2HT-75, Dimethyldi (hydrogenated tallow) ammonium chloride 75% active, 1633602, to the Bluegill Sunfish *Lepomis machrochirus* Rafinesque and Rainbow Trout *Salmo gairdneri* Richardson. Study number 398-001. International Research and Development Corporation.

Other Available Reports

This report was also summarized for rainbow trout.

Other

Last Changed: May 14, 2003
Order number for sorting: 17s [bluegill]

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Test Substance

Identity: Arquad 2HT-75 (CAS RN 61789-80-8;
Dimethyldi (hydrogenated tallow) ammonium chloride)
Purity: 75%
Remarks:

Method

Method/guideline followed: Test procedures followed EPA 1975, Methods for acute toxicity tests with fish, macroinvertebrates and amphibians (EPA 660/3-75-00)

Type: Static acute

GLP: No

Year: 1977

Species/Strain/Supplier: Rainbow trout/NA/commercial supplier

Analytical Monitoring: No

Exposure Period: 96 hours

Statistical Methods: Spearman-Karber LC₅₀ calculations (Finney 1971)

Remarks: The study measured the acute toxicity of the test substance to rainbow trout during a 96-hour static exposure period. Fish were maintained in the laboratory until testing. Water used for holding and testing was reconstituted soft deionized well water having approximately the following: pH 7.6, total hardness 43 mg/l as CaCO₃, total alkalinity 28 mg/l as CaCO₃, and specific conductance 180 ? mhos/cm. Rainbow trout at the time of testing were approximately 4 months old and had a mean length of 50 mm and a mean weight of 1.08 g. Forty-eight hours prior to the test, feeding was ceased. Five exposure levels and a control were used in the test. No replication of test levels was used. Test substance was melted in a hot-water bath, weighed and diluted to volume in volumetric glassware with deionized water. Test vessels were 5-gallon glass containers holding 15 liters of test solution. Tests were initiated by introducing the test substance into the vessels containing dilution water, thoroughly mixing the solutions, then introducing the fish. Ten fish were placed into each test vessel. Fish loading in the test was 0.72 g/l. Observations for deaths and abnormal behavioral effects were made at 24, 48 and 96 hours. Dissolved oxygen and pH were measured regularly through study for the control, low, medium, and high test concentration levels.

Results

Nominal concentrations (mg/l): 0 (control), 1.0, 1.8, 3.2, 5.6 and 10 mg/l
Measured concentrations (mg/l): N/A
Unit: mg/l
Element Value: LC₅₀ (95% confidence intervals could not be calculated due to lack of partial kills)
Statistical Results: 96-hour LC₅₀ = 4.22 mg/l
48-hour LC₅₀ = 4.22 mg/l
24-hour LC₅₀ = 4.22 mg/l
96-hour NOEC = 1.8 mg/l
Results: see above
Remarks: 100% mortality occurred in the 5.6 and 10 mg/l treatments within the first 24 hours. No further mortality occurred. Behavioral observations made during the test indicated that rainbow trout exposed to 3.2 mg/l and higher became stressed and showed signs of dark discoloration. Temperature averaged 12.0 ± 1°C, and the dissolved oxygen concentration and pH during the study ranged from 5.4 to 9.9 mg/l and from 6.93 to 7.55, respectively.

Conclusions

The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Cationics Task Group).

Data Quality

Reliability (Klimisch): 1B
Remarks: Reliable without restriction; comparable to guideline study

References

Dean, W. P. 1977. The Acute Toxicity of Arquad 2HT-75, Dimethyldi (hydrogenated tallow) ammonium chloride 75% Active, 1633602, to the Bluegill Sunfish *Lepomis machrochirus* Rafinesque and Rainbow Trout *Salmo gairdneri* Richardson. Study number 398-001. International Research and Development Corporation.

Other Available Reports

This report was also summarized for bluegill sunfish.

Other

Last Changed: September 4, 2003
Order number for sorting: 17s [trout]
Remarks:

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Test Substance

Identity: Arquad 2HT-75 (CAS RN 61789-80-8;
Ditallowdimethylammoniumchloride, hydrogenated)
Purity: Not stated
Remarks:

Method

Method/guideline followed: OECD Guidelines for Testing of Chemicals,
Guideline No. 203
Type: Static acute
GLP: Yes
Year: 1987
Species/Strain/Supplier: Rainbow trout/not stated/Forellenhof Fredesloh
Analytical Monitoring: No
Exposure Period: 96 hours
Statistical Methods: Graphical plot of percent mortality vs. log concentration
Remarks: The report described the acute toxicity of the test substance to rainbow trout in a static exposure system. Rainbow trout were purchased and held in the laboratory during an adaptation period. During the first 12 days in holding, 7% mortality in the batch of fish occurred. Adaptation was continued for an additional five days with 0.5% mortality during that time. The fish were considered acceptable for testing at that time. During the adaptation period, fish were held in aerated dechlorinated city water under a 12-hour photoperiod. During testing, reconstituted water was used as dilution water. Hardness was not reported. In preparation for the start of the test, test vessels were filled with 10 liters of reconstituted water and aerated for four days. After that period, water temperature, dissolved oxygen and pH were checked every 24 hours. Test substance was weighed and dispersed into a 2-liter beaker and stirred for 2 hours using a magnetic stirrer. Immediately afterward, the mixture was transferred from the beaker into the test vessel, and fish were distributed to each vessel. Each treatment consisted of two replicate vessels each holding five fish. Observations of mortality were made at 1, 24, 48, 72 and 96 hours.

Results

Nominal concentrations (mg/l): 0 (control), 0.7, 1.2, 2.0, 3.5, 6.0, and 10 mg/l
Measured concentrations (mg/l): N/A
Unit: mg/l
Element Value: 96-hour LC₅₀ = 3.4 mg/l

Statistical Results: see above
Result: In addition to the 96-hour LC₅₀ value, the following information was included:
LC₀ = 1.2 mg/l
LC₁₀₀ = 10.0 mg/l
Remarks: 100% mortality occurred within one hour at 10 mg/l. 70% mortality occurred by the end of the test at 6.0 mg/l. While 40% mortality occurred at 2.0 mg/l, no mortality occurred at 3.5 mg/l or at concentrations below 1.2 mg/l (including the control group). Temperature ranged from 14.3 to 14.8°C, dissolved oxygen ranged from 10.0 to 10.3 mg/l and pH remained at 8.1.

Conclusions The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Cationics Task Group).

Data Quality

Reliability (Klimisch): 1A
Remarks: Reliable without restriction; guideline study (OECD)

References

Domröse, A. M. 1987. Investigation of the Lethal Effects of the Test Sample Arquad 2 HT-75 to the Rainbow Trout (OECD 203). NATEC Institute, Hamburg, Germany.

Other Available Reports

Other

Last Changed: April 10, 2003
Order number for sorting: 17t
Remarks:

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Test Substance

Identity: Ditalow dimethyl ammonium chloride (DTDMAC);
(CAS RN 68783-78-8)
Purity: Not stated
Remarks:

Method

Method/guideline followed: Test procedures followed EPA 1975; Methods for acute toxicity tests with fish, macroinvertebrates and amphibians (EPA 660/3-75-009).

Type: Static acute
GLP: No
Year: 1982
Species/Strain/Supplier: Bluegill/*Lepomis macrochirus*/commercial hatcheries
Analytical Monitoring: Yes
Exposure Period: 96 hours
Statistical Methods: Probit analysis or other accepted statistical procedures.
Remarks: The 96-hour tests were conducted in 20-liter glass aquaria containing 15 liters of test solutions. The test waters were maintained at 19-22°C and were not aerated. Ten fish were exposed to each of five test concentrations and a control in reconstituted water or Town River water (Plymouth County, Massachusetts). Chemical and physical quality of the reconstituted water was as follows: pH 6.5 – 7.3; total hardness 131 – 163 mg/l CaCO₃; suspended solids 0 mg/l; chlorinated insecticides < 0.005 µg/l; and organophosphates < 0.01 µg/l. Chemical and physical quality of the Town River water was as follows: pH 6.4 – 7.7; total hardness 14 – 38 mg/l CaCO₃; suspended solids 2 – 84 mg/l; chlorinated insecticides < 0.1 µg/l; organophosphates < 0.5 µg/l; methylene blue active substances 0.04 – 0.59 mg/l; and disulfine blue active substances 0.01 – 0.015 mg/l. Bluegill ranged from 1.2 to 1.7 g in weight and from 23 to 60 mm in length. Fish were acclimated for 14 to 30 days prior to use in water having physical and chemical characteristics similar to those of the water used in the tests. Fish were fed trout chow daily during acclimation, but were not fed 24 hours to 48 hours prior to and during testing. In an additional test, bluegill were exposed to 10.1 ml/l in river water in conjunction with 0-200 mg/l suspended solids (bottom silt collected from the Town River, Plymouth County, Massachusetts). The LC₅₀ values represent nominal concentrations of the active ingredient.

This publication presents data for a number of endpoints and does not specify concentrations used for assay. The value is included in the dataset since it provides information consistent with the data for the category.

Results

Nominal concentrations (mg/l): Not stated
Measured concentrations (mg/l): N/A
Unit: mg/l
Element Value: 96-hour LC₅₀ (95% Confidence Interval, CI)
Statistical Results: 96-hour LC₅₀ in reconstituted water ranged from 0.62 mg/l (0.45 – 0.85) to 3.0 mg/l (CI not reported).
96-hour LC₅₀ in Town River water ranged from 10.1 mg/l (8.3 – 12.6) to >24.0 mg/l (CI not reported).
Result: The addition of suspended solids to Town River water further reduced the bioavailability of the test substance to bluegill exposed to 10.1 mg/l of the test substance. When 20 mg/l of suspended solids were added to the 10.1 mg/l test substance concentration 80% mortality was noted; however, at 50 mg/l of suspended solids and greater, mortality was 0%.

Remarks:

Conclusions

The data are useful in support of the overall category. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Cationics Task Group)

Data Quality

Reliability (Klimisch): 2B
Remarks: Reliable with restriction; basic data given

References

Lewis, M. A. and V. T. Wee. 1983. Aquatic Safety Assessment for Cationic Surfactants. Microbiological Associates, Bethesda, MD, USA. Unpublished report (No. T1806.501).

Other

Last Changed: May 14, 2003
Order number for sorting: 604 [bluegill]
Remarks:

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Test Substance

Identity: Ditalow dimethyl ammonium chloride (DTDMAC);
(CAS RN 68783-78-8)
Purity: Not stated
Remarks:

Method

Method/guideline followed: Test procedures followed EPA 1975; Methods for acute toxicity tests with fish, macroinvertebrates and amphibians (EPA 660/3-75-009).
Type: Static acute
GLP: No
Year: 1982
Species/Strain/Supplier: Sheepshead minnow/*(Cyprinidon variagatus)* /obtained from the Big Lagoon near Pensacola, Florida.
Analytical Monitoring: Yes
Exposure Period: 96 hours
Statistical Methods: Mortality data were analyzed by probit analysis.
Remarks: The test species were acclimated to laboratory test conditions (salinity of 24‰ and pH of 8.0 ± 0.5) for at least one week before use. Tests were conducted in 19-liter glass aquaria containing 15 liters of filtered, natural seawater. Salinity ranged from 16 to 26‰ during testing, and the water temperature was maintained at $20 \pm 1^\circ\text{C}$. Ten sheepshead minnows (15-20 mm) were exposed to each of five test concentrations and the control. Mortality was recorded daily. The LC_{50} values were based on nominal concentrations.

This publication presents data for a number of endpoints and does not specify concentrations used for assay. The value is included in the dataset since it provides information consistent with the data for the category.

Results

Nominal concentrations (mg/l): Not stated
Measured concentrations (mg/l): Not stated
Unit: mg/l
Element Value: 96-hour LC_{50}
Statistical Results: 96-hour $LC_{50} = 24.0$ mg/l
(95% confidence interval of 9.5 – 63.0 mg/l)
Remarks:

Conclusions

The data are useful in support of the overall category.
(American Chemistry Council Fatty Nitrogen Derivatives
Panel, Cationics Task Group)

Data Quality

Reliability (Klimisch):

2B

Remarks:

Reliable with restriction; basic data given

References

Lewis, M. A. and V. T. Wee. 1983. Aquatic Safety
Assessment for Cationic Surfactants. Microbiological
Associates, Bethesda, MD, USA. Unpublished report (No.
T1806.501).

Other

Last Changed:

May 14, 2003

Order number for sorting:

604 b [sheepshead minnow]

Remarks:

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Test Substance

Identity: Dodecyl trimethyl ammonium chloride (C₁₂TMAC);
(CAS RN 112-00-5)
Purity: 35%
Remarks:

Method

Method/guideline followed: U. S. EPA 1975. Methods for Acute Toxicity Tests with Fish, Macroinvertebrates and Amphibians. Committee on Methods for Toxicity Tests with Aquatic Organisms. EPA-660/3-75-009.

Type: Acute static
GLP: Not stated
Year: 1983-1984
Species/Strain/Supplier: *Ceriodaphnia sp.*/Not stated/Not stated
Analytical Monitoring: Not stated
Exposure Period: 48 hours
Statistical methods: Mortality data were analyzed by probit analysis to calculate the LC₅₀ values and associated 95% confidence intervals. Survival was analyzed by chi-square techniques.

Remarks: Water from Acton Lake was used for this test. *Ceriodaphnia sp.* were acclimated to the test conditions for at least two generations before use. *Ceriodaphnia sp.* were fed a diet of baker's yeast. For each test concentration, five neonate *Ceriodaphnia sp.* were placed in 30 ml of test solution in a 50 ml beaker. Three beakers were used per concentration per test. Test solutions were prepared by adding the test substance from a stock solution, prepared in deionized water (without the use of a solvent), to the test water. No aeration was used during the study. Mortality was recorded daily. The pH, and dissolved oxygen content were determined at the beginning and end of the test for one beaker in the control and lowest, middle and highest test concentrations. The LC₅₀ value was based on nominal concentrations of the test substance.

Results

Nominal concentrations (mg/l): Not stated
Measured concentrations (mg/l): Not stated
Unit: mg/l, as active ingredient
Elemental Value: 48-hour LC₅₀ = 0.39 mg/l
(95% confidence interval of 0.35 – 0.43 mg/l)
NOEC (48 hour): Not stated

Remarks: Average (standard deviation, sample size) physiochemical characteristics measured in the Acton Lake water were: Total hardness = 197 mg/l as CaCO₃ (7, 4); pH = 7.3 (0.2, 9); total suspended solids = 9.9 mg/l (3.1, 7); and dissolved oxygen = 9.4 mg/l (0.2, 6).

Conclusions

Remarks: The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Cationics Task Group)

Data Quality

Reliability (Klimisch): 1B
Remarks: Reliable without restriction; comparable to guideline study.

References

Taylor, M. J. 1984. Comparative Sensitivity of *Ceriodaphnia Sp.* and *Daphnia Magna* to Select Surfactants. Procter & Gamble Co., Cincinnati, OH, US. Unpublished report (Notebook: ZE-1154 and ME-1082).

Other Available Reports

Other

Last changed: May 14, 2003
Order number for sorting: 110
Remarks:

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Test Substance

Identity: Monotallowtrimethyl ammonium chloride
(CAS RN 8030-78-2; quaternary ammonium compounds, trimethyltallow alkyl, chlorides)

Purity: non-radiolabeled: 48.4%

Remarks: Stock solutions were prepared using non-radiolabeled test substance and radiolabeled ^{14}C -Alkyl Stearyl trimethyl ammonium chloride (^{14}C -STAC) in isopropanol. Purity of ^{14}C -STAC was 98%

Method

Method/guideline followed: Not stated

Type: Acute

GLP: Not stated

Year: 1980-1981

Species/Strain/Supplier: *Daphnia magna* /Not stated/Not stated

Analytical Monitoring: Yes

Exposure Period: 48 hours

Statistical Methods: The 48-hour LC_{50} values were determined by probit analysis based on the geometric mean of the 0-, 24- and 48-hour concentrations to reflect overall exposure concentrations.

Remarks: Acute toxicity tests were initiated by placing 5 *Daphnia* (<24 hours old) into each of four replicate test chambers for each of the seven concentrations of test substance in river water (total hardness ~300-350 mg/l), control and solvent control (isopropanol, IPA). The river water, exemplifying a natural surface water that received sewage effluent, was collected from the White River (Indiana) and transported for cold storage (~4°C). These tests were run in conjunction with similar tests using water from two other sources (Southwest well water and laboratory blended water), all of which were repeated to ensure reproducibility. The same procedures were utilized in the repeat tests with the exception of testing a more recently collected batch of White River water. There was no renewal of test water throughout the 48-hour test period. Mortality was recorded daily and water chemistry measurements were taken at the beginning and conclusion of the test period for control waters only. Each test material concentration was verified by radiochemical counting of triplicate 10 ml samples collected from the fresh stock solution (0 hour) and from a randomly selected beaker after 24 and 48 hours.

Results

Nominal concentrations (µg/l): 115, 155, 210, 280, 370, 490 and 650

Measured concentrations (µg/l):

Nominal Concentrations (µg/l)	Geometric Mean* of Measured Concentrations (µg/l)
115.0	35.0
155.0	39.0
210.0	57.7
280.0	87.5
370.0	129.6
490.0	162.1
650.0	214.2

* Values in the table represent the geometric mean of the 0-, 24- and 48-hour concentration analyses for initial test only.

Unit:

µg/l

Elemental Value:

24-hour LC₅₀ = 191.7 µg/l (initial test result only)

48-hour LC₅₀ = 98.9 µg/l (initial test result only)

NOEC was not stated

Result:

Nominal concentration (µg/l)	Mortality					
	Initial		Repeated		Repeated	
	24 hr	48 hr	24 hr	48 hr	24 hr	48 hr
Control	2	2	0	0	0	0
IPA control	0	0	0	0	0	0
11.5	0	0	9	13	0	0
15.5	0	0	10	20	0	1
21.0	0	3	18	20	0	0
28.0	1	15	19	20	1	3
37.0	3	20	19	20	0	0
49.0	11	20	20	20	0	0
65.0	20	20	20	20	3	4

Remarks:

Distribution and removal studies were conducted prior to the acute toxicity tests. Because of the very rapid removal of the test substance from the water column, the geometric means of the 0, 24 and 48-hour concentrations were considered to be the overall exposure concentrations in the acute toxicity tests. Water column samples were collected for repeated river water acute test but concentrations were not verified because biological data were stastically unacceptable for probit analysis.

The acute test in river water was repeated using the same concentration range as the initial test. Mortality in this repeat test was 100% at the next to lowest concentration; therefore, the test was repeated a second time utilizing a more recently collected batch of river water and adjusting the concentration range to bracket an LC₅₀ value estimated from the previous test. In this test, no significant mortality occurred at any concentration.

Conclusions

The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Cationics Task Group)

Remarks:

In the initial acute toxicity tests, little difference existed between LC₅₀ values for blended and well waters. The river water LC₅₀, however, was 5 to 11 times higher, possibly related to the presence of solids causing test substance adsorption and reduced bioavailability. An additional factor may have been that the river water contained endogenous nutritional sources perhaps enhancing daphnid resistance to the effects of the test substance.

Data Quality

Reliability (Klimisch):

1B

Remarks:

Reliable without restriction; comparable to guideline study.

References

Valentine, L. C. and W. E. Bishop. 1992. Effects of MTTMAC on the Survival and Reproduction of *Daphnia Magna* in Laboratory Waters and a Natural Surface Water. Procter & Gamble Co., Cincinnati, OH, USA. Unpublished report (Notebook: ME-5004, ME-5007 and ZE-1111).

Other Available Reports

This report was also summarized for laboratory blended water and Southwest well water.

Other

Last Changed:

May 14, 2003

Order Number for Sorting:

301 [river water]

Remarks:

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Test Substance

Identity: Monotallowtrimethyl ammonium chloride
(CAS RN 8030-78-2; quaternary ammonium compounds, trimethyltallow alkyl, chlorides)

Purity: non-radiolabeled: 48.4%

Remarks: Stock solutions were prepared using non-radiolabeled test substance and radiolabeled ¹⁴C-Alkyl Stearyl trimethyl ammonium chloride (¹⁴C-STAC) in isopropanol. Purity of ¹⁴C-STAC was 98%

Method

Method/guideline followed: Not stated

Type: Acute

GLP: Not stated

Year: 1980-1981

Species/Strain/Supplier: *Daphnia magna* /Not stated/Not stated

Analytical Monitoring: Yes

Exposure Period: 48 hours

Statistical Methods: The 48-hour LC₅₀ values were determined by probit analysis based on the geometric mean of the 0-, 24- and 48-hour concentrations to reflect overall exposure concentrations.

Remarks: Acute toxicity tests were initiated by placing 5 *Daphnia* (<24 hours old) into each of four replicate test chambers for each of the seven concentrations of test substance in laboratory blended water (total hardness ~150 mg/l), control and solvent control (isopropanol, IPA). These tests were run in conjunction with similar tests using water from two other sources (Southwest well water and river water), all of which were repeated to ensure reproducibility. There was no renewal of test water throughout the 48-hour test period. Mortality was recorded daily and water chemistry measurements were taken at the beginning and conclusion of the test period for control waters only. Each test material concentration was verified by radiochemical counting of triplicate 10 ml samples collected from the fresh stock solution (0 hour) and from a randomly selected beaker after 24 and 48 hours.

Results

Nominal concentrations (µg/l): 11.5, 15.5, 21.0, 28.0, 37.0, 49.0 and 65.0

Measured concentrations (µg/l):

Nominal concentration (µg/l)	Geometric Mean* of Measured Concentrations (µg/l)	
	Initial	Repeated
11.5	3.3	4.4
15.5	5.3	6.0
21.0	9.0	8.9
28.0	10.6	12.1
37.0	15.7	14.5
49.0	17.4	22.9
65.0	29.5	--

* Values in the table represent the geometric mean of the 0-, 24- and 48-hour concentration analyses for each test.
 -- = concentration level not repeated

Unit:

µg/l

Elemental Value:

24-hour LC₅₀ = 24.2 µg/l
 (36.9 and 11.4 µg/l in the initial and repeat tests, respectively)

48-hour LC₅₀ = 12.6 µg/l
 (16.3 and 8.8 µg/l in the initial and repeat tests, respectively)

NOEC was not stated

Result:

Nominal concentration (µg/l)	Mortality			
	Initial		Repeated	
	24 hr	48 hr	24 hr	48 hr
Control	0	0	0	0
IPA control	0	0	0	2
11.5	0	1	0	0
15.5	0	1	0	2
21.0	0	0	3	13
28.0	0	0	9	16
37.0	0	8	20	20
49.0	3	13	20	20
65.0	6	20	--	--

-- = concentration level not repeated

Remarks:

Distribution and removal studies were conducted prior to the acute toxicity tests. Because of the very rapid removal of the test substance from the water column, the geometric means of the 0, 24 and 48-hour concentrations were considered to be the overall exposure concentrations in the acute toxicity tests. Mortality generally increased in a dose-dependent fashion.

Conclusions

The endpoint has been adequately characterized.
(American Chemistry Council Fatty Nitrogen Derivatives Panel, Cationics Task Group)

Remarks:

In the initial acute toxicity tests, LC₅₀ values for the blended water were similar to those of the Southwest well water, but were approximately six times lower than the LC₅₀ values for river water.

Data Quality

Reliability (Klimisch):

1B

Remarks:

Reliable without restriction; comparable to guideline study.

References

Valentine, L. C. and W. E. Bishop. 1992. Effects of MTTMAC on the Survival and Reproduction of *Daphnia Magna* in Laboratory Waters and a Natural Surface Water. Procter & Gamble Co., Cincinnati, OH, USA. Unpublished report (Notebook: ME-5004, ME-5007 and ZE-1111).

Other Available Reports

This report was also summarized for river water and Southwest well water.

Other

Last Changed:

May 14, 2003

Order Number for Sorting:

301 [laboratory blended water]

Remarks:

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Test Substance

Identity: Monotallowtrimethyl ammonium chloride
(CAS RN 8030-78-2; quaternary ammonium compounds, trimethyltallow alkyl, chlorides)

Purity: non-radiolabeled: 48.4%

Remarks: Stock solutions were prepared using non-radiolabeled test substance and radiolabeled ¹⁴C-Alkyl Stearyl trimethyl ammonium chloride (¹⁴C-STAC) in isopropanol. Purity of ¹⁴C-STAC was 98%

Method

Method/guideline followed: Not stated

Type: Acute

GLP: Not stated

Year: 1980-1981

Species/Strain/Supplier: *Daphnia magna* /Not stated/Not stated

Analytical Monitoring: Yes

Exposure Period: 48 hours

Statistical Methods: The 48-hour LC₅₀ values were determined by probit analysis based on the geometric mean of the 0-, 24- and 48-hour concentrations to reflect overall exposure concentrations.

Remarks: Acute toxicity tests were initiated by placing 5 *Daphnia* (<24 hours old) into each of four replicate test chambers for each of the seven concentrations of test substance in Southwest well water (total hardness ~350 mg/l), control and solvent control (isopropanol, IPA). These tests were run in conjunction with similar tests using water from two other sources (river water and laboratory blended water), all of which were repeated to ensure reproducibility. There was no renewal of test water throughout the 48-hour test period. Mortality was recorded daily and water chemistry measurements were taken at the beginning and conclusion of the test period for control waters only. Each test material concentration was verified by radiochemical counting of triplicate 10 ml samples collected from the fresh stock solution (0 hour) and from a randomly selected beaker after 24 and 48 hours.

Results

Nominal concentrations: 11.5, 15.5, 21.0, 28.0, 37.0, 49.0 and 65.0 µg/l

Measured concentrations (µg/l):

Nominal concentration (µg/l)	Geometric Mean* of Measured Concentrations (µg/l)	
	Initial	Repeated
11.5	2.8	3.9
15.5	3.9	6.1
21.0	5.9	8.6
28.0	8.9	11.8
37.0	14.3	14.4
49.0	19.6	24.3
65.0	29.2	37.9

* Values in the table represent the geometric mean of the 0-, 24- and 48-hour concentration analyses for each test.

Unit:

µg/l

Elemental Value:

24-hour LC₅₀ = 14.2 µg/l (repeated test result only)

48-hour LC₅₀ = 17.5 µg/l

(19.8 and 15.3 µg/l in the initial and repeat tests, respectively).

NOEC was not stated

Result:

Nominal concentration (µg/l)	Mortality			
	Initial		Repeated	
	24 hr	48 hr	24 hr	48 hr
Control	0	1	0	1
IPA control	0	0	0	0
11.5	0	0	0	4
15.5	0	0	0	2
21.0	0	0	0	1
28.0	0	0	3	9
37.0	0	7	7	8
49.0	0	10	19	20
65.0	8	15	20	20

Remarks:

Distribution and removal studies were conducted prior to the acute toxicity tests. Because of the very rapid removal of the test substance from the water column, the geometric means of the 0, 24 and 48-hour concentrations were considered to be the overall exposure concentrations in the acute toxicity tests. Mortality generally increased in a dose-dependent fashion, reaching 100% in the next-to-highest concentration by 48 hours in the repeated study. The LC₅₀ values for the initial and repeated tests in southwest well water were similar.

Conclusions

The endpoint has been adequately characterized.
(American Chemistry Council Fatty Nitrogen Derivatives Panel, Cationics Task Group)

Remarks:

In the initial acute toxicity tests, LC₅₀ values for the Southwest well water were similar to those of the blended water, but were approximately five times lower than the LC₅₀ values for river water.

Data Quality

Reliability (Klimisch):

1B

Remarks:

Reliable without restriction; comparable to guideline study.

References

Valentine, L. C. and W. E. Bishop. 1992. Effects of MTTMAC on the Survival and Reproduction of *Daphnia Magna* in Laboratory Waters and a Natural Surface Water. Procter & Gamble Co., Cincinnati, OH, USA. Unpublished report (Notebook: ME-5004, ME-5007 and ZE-1111).

Other Available Reports

This report was also summarized for river water and laboratory blended water.

Other

Last Changed:

May 14, 2003

Order Number for Sorting:

301 [Southwest well water]

Remarks:

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Test Substance

Identity: Arquad 3.16 (CAS RN 52467-63-7;
Tricetylmethyl ammonium chloride)
Purity: 86.0 %
Remarks:

Method

Method/Guideline followed: OECD Guidelines for Testing of Chemicals, *Daphnia* sp., Acute Immobilization Test and Reproduction Test, Part 1, Procedure 202, adopted 4 April 1984
Test type: Static
GLP: Yes
Year: 1990
Analytical procedures: Yes
Species/Strain: *Daphnia magna*/strain from University of Sheffield and originated from the National Institute for Applied Chemical Research, France
Test details: Static
Statistical methods: Median effect concentrations calculated using the computer program of Stephan; because measure concentrations were not all within 20% of their respective nominal values, EC₅₀ values were calculated using means of measured concentrations
Remarks: Based on the results of a range-finding test, groups of 20 *Daphnia* were exposed to the test substance at nominal concentrations of 0.1, 0.18, 0.32, 0.56 and 1.0 mg/l in a 48-hour static renewal acute toxicity test. Two control groups were included in the test; one was exposed to dilution water alone, and the other to dilution water containing acetone at a concentration of 0.1 ml/l. Duplicate vessels were employed at each level. All glassware used during the test was conditioned to the test substance for approximately 48 hours before use. *Daphnia* were maintained in parthenogenetic culture at the Aquatic Studies Laboratories of Life Science Research since receipt. Observations of the *Daphnia* were made 24 and 48 hours after the start of the test. The appearance of the test substance in water was noted during the test.

Results

Nominal concentrations (mg/l): 0, 0.1, 0.18, 0.32, 0.56 and 1.0 mg/l
Measured concentrations (mg/l): 0, 0.92, 0.157, 0.281, 0.512 and 0.802 mg/l at 48 hours
Unit: mg/l

Elemental Value: Measured EC₅₀ (95% Confidence Interval)
 Results: 24-hour EC₅₀ = 0.21 (0.17 – 0.26 mg/l)
 48-hour EC₅₀ = 0.11 (0.09 – 0.12 mg/l)
 Remarks: Temperature, pH and concentration of dissolved oxygen of the control and test media, measured at the start and end of the tests, ranged from 18.4 to 19.9 °C, 8.18 to 8.41, and 96 to 100 mg/l, respectively. Total hardness as mg/l CaCO₃ and alkalinity as mg/l CaCO₃ ranged from 214 to 224 and 138 to 145, respectively. The sodium:potassium and calcium:magnesium ratios were 4.9:1 and 21.8:1, respectively.

At the start of the test, mean measured concentrations of the test substance were ranging from 121 to 191% of their nominal values. After 48 hours, exposure levels dropped to between 46 to 76% of the starting concentrations. The observed variation in measured concentration was thought to reflect the presence of undissolved test material in the samples. All test concentrations were clear and colorless and remained unchanged during the test. The lowest nominal exposure concentration used in the test (0.1 mg/l) resulted in 30% immobility after 48 hours; the lowest concentration at which there was 100% immobility was 0.32 mg/l. Following is a summary of the cumulative immobility:

Nominal Test Concentration (mg/l)	Cumulative Immobility	
	24 hours	48 hours
0.0	0/20	0/20
0.0 (acetone)	0/20	1/20
0.1	2/20	6/20
0.18	11/20	18/20
0.32	7/20	20/20
0.56	19/20	20/20
1.0	20/20	20/20

At 0.18, 0.32 and 0.56 mg/l, some of the immobile *Daphnia* were floating on the surface of the test dilutions. The pattern of immobility was dose-related.

Conclusions

Remarks: The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Cationics Task Group).

Data Quality

Reliability (Klimisch):

1A

Remarks:

Reliable without restriction; guideline study.

References

Jenkins, C. A. 1990. Arquad 3.16: acute toxicity to *Daphnia magna*. Report number 90/AKL012/0348. Life Science Research Limited, Suffolk, UK.

Other

Last changed:

May 14, 2003

Order number for sorting:

32

Remarks:

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Test Substance

Identity: Ditallow dimethyl ammonium chloride (DTDMAC);
(CAS RN 68783-78-8)
Purity: Not stated
Remarks:

Method

Method/guideline followed: U. S. EPA 1975. Methods for Acute Toxicity Tests with Fish, Macroinvertebrates and Amphibians. Committee on Methods for Toxicity Tests with Aquatic Organisms. EPA-660/3-75-009.

Type: Acute static
GLP: Not stated
Year: 1983
Species/Strain/Supplier: Eastern oyster embryos/(*Crassostrea virginica*);
Mysid shrimp (*Mysidopsis bahia*);
Pink shrimp (*Penaeus duorarum*); and
Blue crabs (*Callinectes sapidus*).
All species were obtained from the Big Lagoon near Pensacola, Florida.
Daphnia magna/obtained from the testing laboratory.

Analytical Monitoring: Yes
Exposure Period: 48 hours for the oyster embryos and *Daphnia magna*; and
96 hours for both species of shrimp and the blue crab.
Statistical Methods: Mortality data were analyzed by probit analysis or other
accepted statistical procedures.
Remarks: Procedures for the 48-hour static test for the oyster are as
follows: Oyster embryos were obtained by induced
spawning of sexually mature individuals. Approximately
50,000 embryos were exposed to each of the five test
substance concentrations and the control in 1-liter glass
aquaria containing 900 ml filtered (5µm) seawater. The
test substance concentrations and the controls were tested
in triplicate. The reduction of the number of normal
embryos that developed to the fully-shelled, straight-hinged
veliger stage was monitored during the 48-hour exposure.
The LC₅₀ values were based on nominal concentrations as
active ingredient.

Procedures for the 96-hour static test for the shrimp and
crab were as follows: The tests were conducted in 19-liter
glass aquaria containing 15 liters of filtered, natural
seawater. Salinity ranged from 16 to 26‰ during testing,
and the water temperature was maintained at 20 ± 1°C for

all tests. Five shrimp (25-40 mm) and five crabs (20-30 mm) were exposed to each of five test concentrations and the control. Mortality was recorded daily.

Procedures for the 48-hour static test for the *Daphnia magna* are as follows: Daphnids used in this test were <24 hours old. Tests were conducted in 250 ml glass beakers containing either 150 or 200 ml test solution. The test vessels were maintained at 19 to 22°C and were not aerated during testing. Mortality of the daphnids in each chamber was recorded daily. Test waters utilized were reconstituted water (two tests) and well water. Chemical and physical qualities of the reconstituted water were as follows: pH 6.5–7.3; total hardness 131–163 mg/l CaCO₃; suspended solids 0 mg/l; chlorinated insecticides < 0.005 µg/l; and organophosphates <0.01 µg/l. Chemical and physical qualities of the well water were as follows: pH 7.1–7.9; total hardness 315–348 mg/l CaCO₃; suspended solids 0 mg/l; chlorinated insecticides < 0.005 µg/l; and organophosphates <0.01 µg/l. The five test substance concentrations, the control and where appropriate the solvent control were done in triplicate.

This publication presents data for a number of species and does not specify concentrations used for assay. The values are included in the dataset since they provide information consistent with the data for the category.

Results

Nominal concentrations (mg/l): Not stated
 Measured concentrations (mg/l): Not stated
 Unit: mg/l as active ingredient
 Elemental Values:

LC₅₀ (48 hour):

Species	Water	48 hour LC ₅₀ (95% confidence limit) *
Eastern oyster embryos	Filtered seawater	2.0 mg/l (1.2 – 3.4 mg/l)
<i>Daphnia magna</i>	Reconstituted	0.19 to 0.48 mg/l
<i>Daphnia magna</i>	Well	1.06 mg/l (0.91 – 1.25 mg/l)

LC₅₀ (96 hour):

Species	Water	96 hour LC ₅₀ (95% confidence limit)
Mysid shrimp	Natural seawater	0.22 mg/l (0.17 – 0.30 mg/l)
Pink shrimp	Natural seawater	36 mg/l
Blue crabs	Natural seawater	> 50 mg/l

NOEC was not stated

Remarks:

Conclusions

The data are useful in support of the overall category.
(American Chemistry Council Fatty Nitrogen Derivatives Panel, Cationics Task Group)

Data Quality

Reliability (Klimisch):

2B

Remarks:

Reliable with restriction; basic data given

References

Lewis, M. A. and V. T. Wee. 1983. Aquatic Safety Assessment for Cationic Surfactants. Microbiological Associates, Bethesda, MD, USA. Unpublished report (No. T1806.501).

Other

Last changed:

May 14, 2003

Order number for sorting:

604

Remarks:

4.3 TOXICITY TO AQUATIC PLANTS (ALGAE)

Test Substance

Identity: Arquad 3.16 (CAS RN 52467-63-7;
Tricetylmethyl ammonium chloride)
Purity: 70.8% (based on R3N content and 87.9% activity)
Remarks:

Method

Method/guideline followed: OECD, EEC and ISO Test Guidelines
Test type: Static
GLP: Yes
Year: 1994
Species/Strain/Source: *Selenastrum capricornutum*
Element basis: Not stated
Exposure period: 96 Hours
Analytical monitoring: Yes
Statistical methods: Not stated
Remarks: Based on the results of a range-finding test, *Selenastrum capricornutum* was exposed to the test substance at nominal concentrations of 0.035, 0.071, 0.142, 0.283 and 0.566 mg/l. The toxicity of the test substance to exponentially growing *Selenastrum capricornutum* was determined over an exposure period of 96 hours. The test was conducted in a mineral salts medium at temperatures ranging from 23.7 to 24.6°C in an illuminate orbital incubator. The pH in the test media varied from 8.2 to 9.1. The test was performed using six replicates for the control and three replicates for each concentration.

Results

Nominal concentrations (mg/l): 0.035*, 0.071, 0.142*, 0.283 and 0.566* mg/l
* Concentrations were only measured for the low, middle and high concentrations.
Measured concentrations (mg/l): 0.03, 0.14 and 0.51 mg/l at 0 hours, respectively.
0.01, 0.03 and 38 mg/l at 96 hours, respectively.
Unit: mg/l, as nominal concentration of active ingredient
Element Value: EC50 (95% Confidence Interval)
Results: 96-hour E_bC_{50} = 0.11 mg/l (0.11 – 0.12 mg/l)
96-hour E_tC_{50} = 0.18 mg/l (0.17 – 0.19 mg/l)
NOEC = 0.04 mg/l
LOEC = 0.07 mg/l
Satisfactory control response: Described below
Statistical results: Described above

Remarks: The test was valid as shown by the E_bC_{50} and E_rC_{50} values of the reference compound, potassium dichromate (0.8 and 1.5 mg/l, respectively), the increase of the extinction of the control over 72 hours by a factor of 16 and by a maximum deviation of the pH of 0.9 units. Chemical analysis, using HPLC, of duplicate samples taken at the beginning of the test indicated that the exposure concentrations were substantially achieved (85 – 99% of the nominal values). The concentrations at the end of the test were strongly decreased (21 – 67% of the nominal values), probably due to adsorption of the test substance to the test flask walls. Thus, EC values were calculated based on the nominal, rather than measured, concentrations.

Conclusions

Remarks: The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Cationics Task Group).

Data Quality

Reliability (Klimisch):

1A

Remarks:

Reliable without restriction, guideline study.

References

Kroon, A. G. M. and Geurts, M. G. J. 1994. Toxicity of Arquad 3.16 to the freshwater alga *Selenastrum capricornutum*. Report no. CRL F94024, T 93-10-03. Akzo Research Laboratories Arnhem, The Netherlands.

Other

Last Changed:

May 14, 2003

Order number for sorting:

34

Remarks:

None

4.3 TOXICITY TO AQUATIC PLANTS (ALGAE)

Test Substance

Identity: Ditalow dimethyl ammonium chloride (DTDMAC);
(CAS RN 68783-78-8)
Purity: Not stated
Remarks:

Method

Method/guideline followed: Payne A. G. And R. H. Hall. 1979. A method for measuring algal toxicity and its application to the safety assessment of new chemicals. In L. L. Marking and R. A. Kimerle, eds., *Aquatic Toxicology*, ASTM STP 667. American Society for Testing and Materials, Philadelphia, PA, pp. 171-180.

Type: Chronic/subchronic
GLP: Not stated
Year: Not stated
Species/Strain/Supplier: Green algae (*Selenastrum capricornutum*);
Blue-green algae (*Microcystis aeruginosa*);
Diatom (*Navicula seminulum*); and
Marine flagellate (*Dunalliella tertiolecta*)

Element Basis: Not stated
Analytical Monitoring: Not stated
Exposure Period: Five days
Statistical Methods: Not stated
Remarks: The freshwater species were cultured following the Algal Assay Procedure (AAP) Bottle Test at starting pH of 7.0 ± 0.1 . Silica (20 mg/L) was added to the diatom mixture. The marine alga was cultured following the Marine Algal Assay Procedure (MAAP) Bottle Test at starting pH of 8.0 ± 0.1 and a salinity of 20‰. All algae were exposed to the cationic surfactants in deionized water containing solvent, and *Selenastrum* and *Microcystis* were also exposed to the surfactants in river water which had been filtered through a 0.45- μm filter or autoclaved to remove indigenous algal species. A control and solvent control were included in all tests.

Results

Nominal concentrations (mg/l): 0, 0.01, 1.0, 10, 50 and 100 mg/l
Measured concentrations (mg/l): Not stated
Unit: mg/l, as active ingredient
Element value:

Results:

Species	Dilution Water	Algistatic Concentration (95% confidence limit)	Algicidal Concentration (mg/l)
<i>Selenastrum capricornutum</i>	Distilled	0.23 mg/l (0.16 – 0.32)	--
	White River (autoclaved)	0.71 mg/l (0.44 – 1.15)	--
	Rapid River (autoclaved)	2.6 mg/l (0.5 – 5.3)	--
	Rapid River (filtered)	> 4.0 mg/l	--
<i>Microcystis aeruginosa</i>	Distilled	0.32 mg/l	--
	White River (autoclaved)	0.21 mg/l	--
<i>Navicula seminulum</i>	Distilled	> 0.5 mg/l = 10.0 mg/l	> 0.5 mg/l = 10.0 mg/l
<i>Dunalliella tertiolecta</i>	Seawater	> 0.5 mg/l = 1.0 mg/l	>1.0 mg/l = 10.0 mg/l

Satisfactory control response: Not stated

Statistical results: See above

Remarks: None

Conclusions

Remarks: The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Cationics Task Group)

Data Quality

Reliability (Klimisch): 2B

Remarks: Reliable with restriction; basic data given.

References

Lewis, M. A. and V. T. Wee. 1983. Aquatic Safety Assessment for Cationic Surfactants. Microbiological Associates, Bethesda, MD, USA. Unpublished report (No. T1806.501).

Other

Last changed: May 14, 2003

Order number for sorting: 604

Remarks:

4.3 TOXICITY TO AQUATIC PLANTS (ALGAE)

Test Substance

Identity: Ditallow dimethyl ammonium chloride (DTDMAC);
(CAS RN 68783-78-8)

Purity: 97.7%

Remarks: The test was conducted with pure distearyl dimethyl ammonium chloride. The test substance was specially synthesized to ensure the absence of MTTMAC

Method

Method/guideline followed: Horning, W. B. and C. I. Weber. 1985. Short-term Methods for Estimating the Chronic Toxicity of Effluents and Receiving Waters to Freshwater Organisms. EPA-600/4-85-014. U. S. EPA, Cincinnati, Ohio.

Type: Static

GLP: Yes

Year: 1987-1988

Species/Strain/Supplier: Green algae (*Selenastrum capricornutum*)/Not stated

Element Basis: 10^6 cells

Analytical Monitoring: Yes

Exposure Period: Four days

Statistical methods: Probit analysis was used to calculate the lethal concentrations. For nonquantal data, effective concentrations causing a 20 percent decrease in the appropriate population level parameter and the associated 95% confidence intervals were calculated by nonlinear multiple regression analysis on SAS.

Remarks: Acidic methanol was used as a carrier solvent in the toxicity test due to the low water solubility of the test substance. A solvent control group was included with each toxicity test. Filtered Little Miami River water was used for all tests (pH of 8.1–8.4, hardness of 171 mgCO₃/L, alkalinity of 113 mgCO₃/L, and total organic carbon of 5.4 mg/L). The algal toxicity test was initiated by placing 10^6 cells from a culture in logarithmic phase growth into 100 ml of the test solution. Test solutions were continually stirred (100 rpm) at 25°C with constant illumination of approximately 400 ft-c cool white fluorescent light. At 96 hours, the concentration of algal cells in the test solutions was determined manually with a hemocytometer. Toxicity was manifested as a decrease in cell numbers as compared to the controls.

Results

Nominal concentrations (mg/l): Not stated
Measured concentrations (mg/l): 0, 0.6, 10, 4.2, 9.9 and 16.4 mg/l
Unit: mg/l
Element value: EC₅₀ (95% confidence interval)
Results: 48-hour EC₅₀ = 1.53 mg/l (1.01 – 2.30 mg/l)
96-hour EC₅₀ = 1.12 mg/l (0.756 – 1.67 mg/l)
NOEC was not stated

Satisfactory control response: Yes
Statistical results: See above.
Remarks: The four day algistatic concentration, was > 16.4 mg/l. Algal populations exposed to solvent control concentrations of 32 and 125 µl/l had increased growth relative to the blank control algal populations. The concentrations of solvent used in the test substance exposure groups ranged from 3 to 125 µl/l. A dose-dependent decrease in algal growth was observed in the test substance exposure groups.

Conclusions

Remarks: The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Cationics Task Group)

Data Quality

Reliability (Klimisch): 1B
Remarks: Reliable without restriction; comparable to guideline study.

References

Shorter, S. J. 1993. The Chronic Effects of DTDMAC on the Fathead Minnow (*Pimephales promelas*) Larval Survival and Growth. Procter & Gamble Co., Cincinnati, OH, USA. Unpublished report (Report No. E89-006).

Other

Last changed: May 14, 2003
Order number for sorting: 605
Remarks:

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

Test Substance

Identity: Monotallowtrimethyl ammonium chloride
(CAS RN 8030-78-2; quaternary ammonium compounds, trimethyltallow alkyl, chlorides)

Purity: non-radiolabeled: 48.4%

Remarks: Stock solutions were prepared using non-radiolabeled test substance and radiolabeled.
¹⁴C-Alkyl Stearyl trimethyl ammonium chloride (¹⁴C-STAC) in isopropanol. Purity of ¹⁴C-STAC was 98%.

Method

Method/Guideline followed: Not stated

Test type: Static (daily renewal)

GLP: Not stated

Year: 1980-1981

Analytical procedures: Yes

Species/Strain: *Daphnia magna*/Not stated

Test details: Static daily renewal

Statistical methods: Mortality data were analyzed by probit analysis to derive a 21-day LC₅₀ value and associated 95% confidence interval. T-tests were used to analyze statistically significant differences in other tested parameters including days to first reproduction, total young production, mean brood size, and 21-day length.

Remarks: *Daphnia magna* (< 24 hours old) were exposed to six concentrations of the test substance in a 21-day static-daily renewal test using river water (total hardness ~300-350 mg/l). The river water, exemplifying natural surface water that received sewage effluent, was collected from the White River (Indiana) and transported for cold storage (~4°C). Control and isopropanol control (IPA) groups were also evaluated. The test was also conducted in laboratory blended water and Southwest well water; the laboratory blended water test was discontinued after 14 days due to inadequate reproduction by control organisms. Mortality was monitored daily and the number of young produced in each beaker was recorded after which they were discarded. Temperature was recorded daily and pH, dissolved oxygen and hardness were determined on alternate days in control waters, both fresh and 24 hours old. Daphnid length was also determined on day 21 by the use of an ocular micrometer measuring from the base of the spine to the apex of the helmet.

Results

Nominal concentrations: 74.4, 110.4, 146.4, 218.4, 290.4, 578.4 µg/l
 Measured concentrations: 35.7, 53.4, 68.3, 99.1, 122.3 and 309.3 µg/l
 (Geometric means of the 0- and 24-hr analyses)
 Unit: µg/l
 Elemental Values: 21-day LC₅₀ = 190.0 µg/l
 NOEC = 99.1 µg/l
 LOEC = 122.0 µg/l
 Remarks: Distribution and removal studies were conducted prior to the acute toxicity tests. Because of the very rapid removal of the test substance from the water column, the geometric means of the 0- and 24-hour concentrations was considered to be the overall exposure concentrations in the chronic toxicity tests. The water chemistry remained relatively constant during the test periods. Dissolved oxygen far exceeded daphnid oxygen demand throughout the study.

Water Chemistry Parameter	Mean Value*
Daily Temperature (°C)	20.2 ± 1.0
pH (range)	(7.5 – 8.3)
Total Hardness (as mg CaCO ₃ /L)	348 ± 16
Dissolved Oxygen (mg/L)	9.0 ± 0.2

* Means were reported unless otherwise noted.

Reproduction was first observed by Day 8 or 9 for all but the highest concentration (309.3 µg/l) in the chronic river water tests.

White River Water Test				
Measured Concentration (µg/l)	% Mortality	Total Young Produced	Mean Brood Size	21-Day Length (mm)
Control	5	1292	10	3.6
IPA Control	5	1365	12	3.5
35.7	5	1295	11	3.6
53.4	5	1292	10	3.4
68.3	0	1292	10	3.4
99.1	0	1107	9	3.2
122.0	20	1049*	11	3.2
309.3	100*	--	--	--

* Significantly different from IPA control (p < 0.05)

-- = not applicable due to 100% mortality

Conclusions

Remarks: The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Cationics Task Group)

Data Quality

Reliability (Klimisch): 1B
Remarks: Reliable without restriction; comparable to guideline study.

References

Valentine, L. C. and W. E. Bishop. 1992. Effects of MTTMAC on the Survival and Reproduction of *Daphnia Magna* in Laboratory Waters and a Natural Surface Water. Procter & Gamble Co., Cincinnati, OH, USA. Unpublished report (Notebook: ME-5004, ME-5007 and ZE-1111).

Other Available Reports

This report was also summarized for Southwest well water.

Other

Last changed: May 14, 2003
Order number for sorting: 301 [river water]
Remarks:

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

Test Substance

Identity: Monotallowtrimethyl ammonium chloride
(CAS RN 8030-78-2; quaternary ammonium compounds, trimethyltallow alkyl, chlorides)

Purity: non-radiolabeled: 48.4%

Remarks: Stock solutions were prepared using non-radiolabeled test substance and radiolabeled.
¹⁴C-Alkyl Stearyl trimethyl ammonium chloride (¹⁴C-STAC) in isopropanol. Purity of ¹⁴C-STAC was 98%.

Method

Method/Guideline followed: Not stated

Test type: Static (daily renewal)

GLP: Not stated

Year: 1980-1981

Analytical procedures: Yes

Species/Strain: *Daphnia magna*/Not stated

Test details: Static daily renewal

Statistical methods: Mortality data were analyzed by probit analysis to derive a 21-day LC₅₀ value and associated 95% confidence interval. T-tests were used to analyze statistically significant differences in other tested parameters including days to first reproduction, total young production, mean brood size, and 21-day length.

Remarks: *Daphnia magna* (< 24 hours old) were exposed to six concentrations of the test substance in a 21-day static-daily renewal test using Southwest well water (total hardness ~350 mg/l). Control and isopropanol control (IPA) groups were also evaluated. The test was also conducted in laboratory blended water river water; the laboratory blended water test was discontinued after 14 days due to inadequate reproduction by control organisms. Mortality was monitored daily and the number of young produced in each beaker was recorded after which they were discarded. Temperature was recorded daily and pH, dissolved oxygen and hardness were determined on alternate days in control waters, both fresh and 24 hours old. Daphnid length was also determined on day 21 by the use of an ocular micrometer measuring from the base of the spine to the apex of the helmet. Because no statistically significant differences in Daphnid length occurred as a result of exposure to increasing concentrations of the test substance, this parameter was not measured in the well water.

Results

Nominal concentration: 2.5, 5.0, 10.0, 20.0, 40.0 and 80.0 µg/l
 Measured concentrations: 1.6, 3.1, 6.8, 14.6, 30.6 and 60.8 µg/l
 (Geometric means of the 0- and 24-hr analyses)
 Unit: µg/l
 Elemental Values: 21-day LC₅₀ = 22.7 µg/l
 NOEC = 6.8 µg/l
 LOEC = 16.4 µg/l
 Remarks: Distribution and removal studies were conducted prior to the acute toxicity tests. Because of the very rapid removal of the test substance from the water column, the geometric mean of the 0- and 24-hour concentrations was considered to be the overall exposure concentration in the chronic toxicity tests. The water chemistries remained relatively constant during the test periods. Dissolved oxygen far exceeded daphnid oxygen demand throughout the study.

Water Chemistry Parameter	Mean Value *
Daily Temperature (°C)	20.6 ± 1.1
pH (range)	(8.4 – 8.8)
Total Hardness (as mg CaCO ₃ /L)	342 ± 7
Dissolved Oxygen (mg/L)	8.1 ± 1.1

* Means were reported unless otherwise noted.

Reproduction was first observed on Day 11 for all but the highest concentration (60.3 µg/l) in the chronic Southwest well water tests.

Southwest well water test			
Measured Concentration (µg/l)	% Mortality	Total Young Produced	Mean Brood Size
Control	10	690	7
IPA Control	5	699	7
1.6	10	670	7
3.1	6	531	6
6.8	15	649	7
14.6	42	384 *	6
30.6	50 *	509 *	10
60.3	100 *	--	--

* Significantly different from IPA control (p< 0.05)

-- = not applicable due to 100% mortality

Conclusions

Remarks: The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Cationics Task Group)

Data Quality

Reliability (Klimisch): 1B
Remarks: Reliable without restriction; comparable to guideline study.

References

Valentine, L. C. and W. E. Bishop. 1992. Effects of MTTMAC on the Survival and Reproduction of *Daphnia Magna* in Laboratory Waters and a Natural Surface Water. Procter & Gamble Co., Cincinnati, OH, USA. Unpublished report (Notebook: ME-5004, ME-5007 and ZE-1111).

Other Available Reports

This report was also summarized for river water.

Other

Last changed: May 14, 2003
Order number for sorting: 301 [Southwest well water]
Remarks: