Section A7.1.1.1.1 Annex Point IIA VII.7.6.2.1	Hydrolysis as a function of pH and identification of breakdown products	
	1 REFERENCE	Official use only
1.1 Reference	Haag, W.R. et al. (1988a), Estimation of Hydrolysis Rate Constants for Acrolein (Magnacide®H Herbicide, Magnacide®B Microbiocide) in the Environment, SRI International, SRI Project No. 3562-3.	
1.2 Data protection	Yes	
1.2.1 Data owner	Baker Petrolite	
1.2.2 Criteria for data protection	Data on new a.s. for first entry to Annex I	
	2 GUIDELINES AND QUALITY ASSURANCE	
2.1 Guideline study	Yes US EPA-FIFRA, Subdivision N, Guideline 161-1	
2.2 GLP	Yes	
2.3 Deviations	No	
	3 MATERIALS AND METHODS	
3.1 Test material	As given in Section 2	
3.1.1 Lot/Batch number	NN-481-76	
3.1.2 Specification	As given in Section 2	
3.1.3 Purity	See 3.1.2	
3.1.4 Further relevant properties		
3.2 Reference substance	No	
3.2.1 Initial concentration of reference substance		
3.3 Test solution	See Tables A7_1_1_1_1-1 and A7_1_1_1_1-2	
3.4 Testing procedure		
3.4.1 Test system	See Table A7_1_1_1_1-3	
3.4.2 Temperature	25°C	

Section A7.1.1.1.1 Annex Point IIA VII.7.6.2.1	Hydrolysis as a function of pH and identification of breakdown products	
3.4.3 pH	(table below)	

EXPERIMENTAL CONDITIONS FOR DETERMINING ACROLEIN HYDRATION RATE CONSTANTS

Run	pH	$[Acrolein]_0$ ppm	Water, or Buffer Type	Method
1	0.0	20	1.0 N $HClO_4$	UV-10
2	0.97	5	0.1 N $HClO_4$	UV-1c
3	1.78	40	100 mM phosphate	UV-10
4	3.28	10	10 mM phosphate	UV-1
5	5.37	10	10 mM phosphate	HPLC
6	6.22	10	10 mM phosphate	HPLC
7	7.23	10	10 mM phosphate	HPLC
8	7.2	10	10 mM phosphate	UV-1
9	7.2	10	10 mM phosphate	UV-1
10	8.19	10	10 mM phosphate	HPLC
11	8.67	10	10 mM phosphate	HPLC
12	9.25	10	10 mM phosphate	HPLC
13	10.07	5	10 mM phosphate	UV-1c
14	10.98	5	10 mM phosphate	UV-1c
15	12.00	10	0.01 N NaOH	HPLC
16	12.11	5	0.01 N NaOH	UV-1c
17	5.65	10	pure water	UV-1
18	7.34	10	2 mM phosphate	UV-1
19	7.03	20	100 mM phosphate	UV-10
20	7.75	10	10 mg/L humic acid	UV-1
21	7.99	10	Seawater	UV-1
22	8.46	10	Kansas River	UV-1
23	5.28	30	10 mM phosphate	UV-1
24	7.19	30	10 mM phosphate	UV-1
25	8.74	30	10 mM phosphate	UV-1
26	8.92	30	10 mM phosphate	UV-1

Figure 1: Experimental Conditions for Determining Acrolein Hydration Rate Constants

3.4.4 Duration of the test	Up to 290 hours	
3.4.5 Number of replicates	Duplicate analyses run on each sample	
3.4.6 Sampling	Method UV-1c Solutions were placed into 1 cm spectrophotometer cells thermostatted at 25 ± 1°C and the reaction monitored continually by UV absorbance at 210 nm. This method was the most convenient and precise and was used whenever the reaction could be completed within 24 hours (pH extremes). Method UV-10	

Section A7.1.1.1.1 **Annex Point IIA VII.7.6.2.1**	**Hydrolysis as a function of pH and identification of breakdown products**	
	Solutions were placed into 10 cm spectrophotometer cells and the absorbance at 320 nm measured periodically. Between measurements the cells were stored at 25°C in the dark. This method was used in three early experiments before the other more sensitive analytical methods were developed. Method UV-1 Solutions were prepared in volumetric flasks, placed into a dark water bath at 25 ± 0.2°C, and aliquots removed periodically for UV analysis at 218 nm in a 1 cm cell. This method was the most convenient for reactions taking longer than 24 hours. A wavelength of 218 nm was chosen to minimise background absorbance in solutions of humic acid and natural waters. In principle, any wavelength near the acrolein maximum of 210 nm could have been used. Method HLPC Samples were prepared in volumetric flasks, placed into a dark water bath at 25 ± 0.2 °C, and aliquots removed periodically and the reaction stopped by cooling to 1 °C. Samples were stored at 1°C in the dark and analysed at the end of the reaction by HPLC as described below. The small error introduced by incomplete stoppage of the reaction at 1 °C was corrected for by adding the rate constant observed at 1°C. This method was used initially for reactions taking longer than 24 hours, before the more convenient method UV-1 as developed. In particular, the HPLC method was used in Run number 15 to determine the amount of acrolein remaining at equilibrium.	
3.4.7 Analytical methods	HPLC analyses for kinetic runs were performed on a HP 1090 system equipped with a diode array detector. Conditions were as follows: Column: 3 µm Hypersil C18 60 mm x 4.5 mm Eluent: 20% acetonitrile in water at 0.4 ml/min Injection volume: 15 µl Detection: 210 nm Acrolein retention time: 2.5 minutes Quantitation was by external standards; peak areas varied linearly with concentration over the range of 1-100 ppm with a correlation coefficient > 0.999. Absorbance measurements for kinetic runs were made on HP 8450 UV/VIS spectrophotometer. Acrolein absorbance obeyed Beer's law with an extinction coefficient of 11,800 M^{-1} cm^{-1} over the concentration range studied. A similar calibration curve was found at 328 nm, also with a correlation coefficient greater than 0.999. Product analyses were performed using HPLC GC/ECD and GC/MS following the derivitisation with PFPH. Aqueous samples (1.0 ml) were mixed with 1.0 ml of a solution of 1.53 g/l pentaflurophenylhydrazine (PFPH) (12) in methanol and allowed to react overnight at 1 °C in the dark. At pH > 7, the PFPH derivative of 3-hydroxypropanal was unstable and therefore for samples at pH 9, 24 µl of 0.50 M pH 4 phosphate buffer was added to the derivitising mixture to bring the pH to 6. The PFPH derivative of acrolein was similarly unstable at pH > 5 and therefore acrolein was determined directly by ultraviolet	

Section A7.1.1.1.1 Annex Point IIA VII.7.6.2.1		Hydrolysis as a function of pH and identification of breakdown products	
		spectrometry at 210 nm on a separate, underivatised aliquot. In each case, the reference cell contained buffer at the same pH as the reaction solution but without acrolein. The data were analysed using the general kinetic rate law for a reversible first order reaction. Statistical analysis was performed using the Statworks® statistics programme.	
3.5	**Preliminary test**	Yes 0.5M phosphate buffer used	
		4 RESULTS	
4.1	**Concentration and hydrolysis values**	See Table A7_1_1_1_1-4	
4.2	**Hydrolysis rate constant (k_h)**		
4.3	**Dissipation time**	See Table A7_1_1_1_1-5	
4.4	**Concentration - time date**		
4.5	**Specification of the transformation products**	See Table A7_1_1_1_1-6	
		5 APPLICANT'S SUMMARY AND CONCLUSION	
5.1	**Materials and methods**	US EPA-FIFRA, Subdivision N, Guideline 161-1. Hydrolysis was studied in a variety of water types and over a broad pH range, in order to gain fundamental kinetic data and allow confident prediction of rates under varying conditions.	
5.2	**Results and discussion**	Acrolein hydration in water is catalysed by both hydrogen and hydroxide ions$^-$, but neither process is expected to be very significant in the natural water pH range of 5 to 9. However, unidentified catalysts, probably including both organic and inorganic compounds, are ubiquitously present in natural waters in sufficient quantities to increase the hydration rate at pH 5 to 9 by an order of magnitude over that observed in pure water. The catalytic effect appears to be quite constant over a broad range of water types and therefore the measured half-lives of 14 to 92 hours (pH 9.3 to 5.3, respectively) are expected to generally be applicable.	
5.2.1	k_H		
5.2.2	DT_{50}	See Table A7_1_1_1_1-5	X
5.2.3	r^2		
5.3	**Conclusion**	The major hydration product is 3-hydroxypropanal, which could not be distinguished from its hydrated form, 3,3-dihydroxy-1-propanol. At 25°C, 9.1 ± 1.5% of acrolein remains at equilibrium. The reversibility of the hydration reaction implies that a small fraction of acrolein will persist for reaction times much longer than the hydration half-life, in the absence of other loss processes. Because volatisation of acrolein is a significant aquatic fate process in turbulent waters, hydration products	

Section A7.1.1.1.1 Annex Point IIA VII.7.6.2.1	Hydrolysis as a function of pH and identification of breakdown products	
	may simply act as a reservoir of acrolein to slow down the volatilisation process. However, in calm waters where volatisation is less important, sorption of acrolein and biotransformation of the hydrated products may drive the reaction to completion, as has been observed previously in irrigation supply waters.	
5.3.1 Reliability	1	
5.3.2 Deficiencies	No	
	Evaluation by Competent Authorities	
	Use separate "evaluation boxes" to provide transparency as to the comments and views submitted	
	EVALUATION BY RAPPORTEUR MEMBER STATE	
Date	30/11//2007	
Materials and Methods	The Applicant's version is considered to be acceptable	
Results and discussion	The Applicant's version is considered to be acceptable with the following amendment. **5.2.2** Table A7_1_1_1_1-5 should be replaced with the following (corrected values underlined);	

Table A7_1_1_1_1-5: Average half life (hours) of parent compound, and dissipation time (hours) of transformation product at pH 5.3, pH 7.2 and pH 9.3

	pH 5.3		pH 7.2		pH 9.3	
	DT_{50}	DT_{90}	DT_{50}	DT_{90}	DT_{50}	DT_{90}
Parent compound (acrolein)	92	>209	37	209	14	>65.8
Transformation product	100	>209	<48	>209	18.5	>65.8

Conclusion	The Applicant's version is considered to be acceptable.	
Reliability	1	
Acceptability	Acceptable	
Remarks	All endpoints and data presented in the summary have been checked against the original study and are correct.	
	COMMENTS FROM ...	
Date	*Give date of comments submitted*	
Materials and Methods	*Discuss additional relevant discrepancies referring to the (sub)heading numbers and to applicant's summary and conclusion.* *Discuss if deviating from view of rapporteur member state*	
Results and discussion	*Discuss if deviating from view of rapporteur member state*	
Conclusion	*Discuss if deviating from view of rapporteur member state*	

Section A7.1.1.1.1 Annex Point IIA VII.7.6.2.1	Hydrolysis as a function of pH and identification of breakdown products	
Reliability	*Discuss if deviating from view of rapporteur member state*	
Acceptability	*Discuss if deviating from view of rapporteur member state*	
Remarks		

Table A7_1_1_1_1-1: Type and composition of buffer solutions

pH	Type of buffer (final molarity)	Composition
5	Phosphate	2 ml of 0.5 M buffer stock solution made up to 100 ml with water
7	Phosphate	2 ml of 0.5 M buffer stock solution made up to 100 ml with water
9	Phosphate	2 ml of 0.5 M buffer stock solution made up to 100 ml with water

Table A7_1_1_1_1-2: Description of test solution

Criteria	Details
Purity of water	Filter-sterilised
Preparation of test medium	Stock solution was prepared by adding neat acrolein to unbuffered Milli-Q purified water. Typically a 200ppm solution was prepared by dissolving 11.9 µl of acrolein in 50 ml of pure water, and a 1000ppm solution by mixing 29.8 µl of acrolein with 25 ml of pure water. The stock solutions were usually prepared daily, stored at 2ºC and discarded after two days.
Test concentrations (mg a.i./l)	5 ppm or 10 ppm
Temperature (°C)	25 ± *0.2*
Controls	2.0 ml of 5.0 M phosphate buffer diluted up to 100 ml.
Identity and concentration of co-solvent	None
Replicates	Duplicate analyses were run on each sample, but one sample per time point was adequate because of the excellent reproducibility of the UV and HPLC measurements.

Table A7_1_1_1_1-3: Description of test system

Glassware	Glass cuvettes, 1 cm and 10 cm
Other equipment	Not specified
Method of sterilisation	Reaction vessels were usually autoclaved to prevent microbial transformation; however, runs using unsterilised glassware were considered equally valid because duplicate runs at certain pH values showed no effect of autoclaving.

Table A7_1_1_1_1-4: Hydrolysis of test compound, transformation products and reference substance, expressed as percentage of initial concentrations, at pH 5, pH 7 and pH 9

pH 5 (5.28)

Compound	Sampling times (*hours*)							
	0	**48**	**76**	**100**	**122**	**144**	**168**	**209**
Parent compound (acrolein)	100	-----	63	50	44	40	36	29
Transformation product (3-hydroxypropanal)	0	29	40	47	57	63	66	71
Total % recovery	100	-----	103	97	101	103	102	100

pH 7 (7.19)

Compound	Sampling times (*hours*)							
	0	**48**	**76**	**100**	**122**	**144**	**168**	**209**
Parent compound (acrolein)	100	-----	25	19	16	16	11	8
Transformation product (3-hydroxypropanal)	0	60	73	77	83	81	82	87
Total % recovery	100	-----	98	96	99	97	93	95

pH 9 (8.92)

Compound	Sampling times (*hours*)						
	0	**3.8**	**18.5**	**28**	**43**	**51.7**	**65.8**
Parent compound (acrolein)	97	90	60	47	32	26	19
Transformation product (3-hydroxypropanal)	3	14	44	56	69	76	79
Total % recovery	100	104	104	103	101	102	98

Table A7_1_1_1_1-5: Dissipation times (hours) of parent compound, transformation products and reference compound at pH 5, pH 7 and pH 9

	pH 5		**pH 7**		**pH 9**	
	DT_{50}	**DT_{90}**	**DT_{50}**	**DT_{90}**	**DT_{50}**	**DT_{90}**
Parent compound (acrolein)	100	>209	76	209	28	>65.8
Transformation product	100	>209	<48	>209	18.5	>65.8

Table A7_1_1_1_1-6: Specification and amount of transformation products

CAS-Number	***CAS and/or IUPAC* Chemical Name*(s)***	**Amount [%] of parent compound measured at**		
		pH 5	**pH 7**	**pH 9**
	3-hydroxypropanal	71	87	79

Section A7.1.1.1.2 Annex Point IIA7.1.1.1.2	Phototransformation in water including identity of transformation products	
	1 REFERENCE	Official use only
• Reference	Haag, W.R. et al. (1988b) Estimation of Photolysis Rate Constants for Acrolein (Magnacide®H Herbicide and Magnacide®B Microbiocide) in the Environment, SRI International, SRI Project No. 3562-3.	
1.1 Data protection	Yes	
1.1.1 Data owner	Baker Petrolite	
1.1.2 Criteria for data protection	Data on new a.s. for first entry to Annex I	
	2 GUIDELINES AND QUALITY ASSURANCE	
2.1 Guideline study	Yes FR 796.3700 and Pesticide Assessment Guidelines, Subdivision N, 161-2	
2.2 GLP	Yes	
2.3 Deviations	No	X
	3 METHOD	
• Test material	As given in Section 2	
3.1.1 Lot/Batch number	NN-481-76	
3.1.2 Specification	As given in Section 2	
3.1.3 Purity	96.2 %	
3.1.4 Radiolabelling	Not used	
3.1.5 UV/VIS absorption spectra and absorbance value	Extinction coefficients were estimated relative to the maximum of 11,800 M^{-1} cm^{-1} at 210 nm using the respective attenuations	
3.1.6 Further relevant properties	None	
3.2 Reference substance	No	
3.2.1 Initial concentration of reference substance		
3.3 Test solution	See Table A7_1_1_1_2-1	
3.4 Testing procedure		
3.4.1 Test system	Sunlight irradiations were performed in screw-capped, 11-mm o.d. quartz tubes, held on a rack at about 30° to the horizon on the roof of the SRI Physical Sciences building on consecutive cloudless days from 6 July to 10 July 1987 (kinetic studies) and from 26 May to 3 June 1988 (product studies). Photolyses were run at ambient temperature, which was 25 ± 5 °C. The actinometer solution (10 µM p-nitroacetophenone/20 mM pyridine) was irradiated in identical fashion and sampled at the same time as the acrolein solutions. Controls consisted of replicate solutions	

Section A7.1.1.1.2 Annex Point IIA7.1.1.1.2		Phototransformation in water including identity of transformation products	
		placed in tubes and in the sun but covered with aluminium foil. During analysis the tubes were sampled at regular intervals and replaced on the rack.	
3.4.2	Properties of light source	See Table A7_1_1_1_2-2	X
3.4.3	Determination of irradiance	A sunlight actinometer was used for kinetic studies. The solution contained 10 µM p-nitroacetophenone and 20 mM pyridine.	
3.4.4	Temperature	25 ± 5 °C	X
3.4.5	pH	7	
3.4.6	Duration of test	Kinetic studies: 4 days Product studies: 8 days	
3.4.7	Number of replicates	Not specified	
3.4.8	Sampling	Samples were stored at 1 °C before analysis. Samples were taken at 0, 18, 42, 66 and 90 hours.	
3.4.9	Analytical methods	Reaction solutions for kinetic runs were prepared by diluting 1.0 ml of 1000 ppm acrolein stock and 2 ml of 0.5 M phosphate buffer to 100 ml with Milli-Q water to yield 10 ppm acrolein and 10 mM phosphate. Runs were performed at pH 3, where the dark hydration reaction is the slowest, at pH 7, which is more typical of natural waters. Solutions of 10 ppm acrolein in 10 mg/l humic acid were prepared by diluting 0.5 ml of 1000 ppm acrolein stock, 5 ml of 100 mg/l humic acid stock and 1.0 ml of 0.5 M pH 7 phosphate buffer to 50 ml. The actinometer solution was prepared by diluting 0.5 ml of PNAP stock and 161 µl of pyridine to 100 ml with Milli-Q water. Solutions for product studies were prepared as for kinetic studies except that 3.0 ml of acrolein stock was used, yielding a final concentration of 30 ppm. Product studies were run only at pH 7, and no actinometer was used. During kinetic studies, acrolein was determined by HPLC on a HP 1090 system equipped with a diode array detector. Conditions were as follows: Column: 3 µm hypersil C18 60 mm x 4.5 mm Eluent: 20 % acetonitrile in water at 0.4 mL/min. Injector volume: 15 µl Detection: 210 nm Acrolein retention time: 2.7 min. Quantitation was achieved by the external standard method. During product studies, acrolein was analysed by direct UV spectrophotometry on a HP 8450 UV/VIS spectrophotometer. The hydration product, 3-hydroxypropanal, was analysed by HPLC following derivatisation with pentafluorophenylhydrazine (PFPH). Conditions were as follows: Column: 3 µm hypersil C18 60 mm x 4.5 mm Eluent: 40 % acetonitrile in water for 3.8 min. increasing to	

Section A7.1.1.1.2 Annex Point IIA7.1.1.1.2	Phototransformation in water including identity of transformation products	
	70 % acetonitrile at 4.1 minutes. Injection volume: 5 µl Detection: 260 nm Retention times: 4.7, 7.5 and 7.8 min. for derivatives of 3-hydroxypropanal, acrolein and propanal, respectively. The retention time of PFPH-derivatised 3-hydroxypropanal was verified by use of a standard prepared by allowing a 30 ppm solution acrolein to hydrate at pH 7 for 40 days. In lieu of an authentic standard for PFPH-derivatised 3-hydroxypropanal, PFPH-derivatised propanal was used as a quantitative standard and assumed that the molar absorptivities of the two derivatives are identical. Statistical analyses were performed using the Statworks® statistical program.	
3.5 Transformation products	Yes	
3.5.1 Method of analysis for transformation products	3-hydroxypropanal was analysed by HPLC following derivatisation with PFPH.	
	4 RESULTS	
4.1 Screening test	Not performed See Table A7_1_1_1_2-3	
4.2 Actinometer data	See Table A7_1_1_1_2-4	
4.3 Controls		
4.4 Photolysis data		
4.4.1 Concentration values		
4.4.2 Mass balance		
4.4.3 k^c_p	0.01 d^{-1}	
4.4.4 Kinetic order		
4.4.5 k^c_p / k^a_p		
4.4.6 Reaction quantum yield (ϕ^c_E)	≤ 0.001	
4.4.7 k_{pE}		
4.4.8 Half-life ($t_{1/2E}$)	70 days	
	5 APPLICANT'S SUMMARY AND CONCLUSION	
5.1 Materials and methods	The study was performed according to the protocols in Federal Register 1985, 50(188) 796.3700, 796.3780,796.3800 and Pesticide Assessment Guidelines, Subdivision N, 161-2, 161-3, 161-4, Report PB83-153973 (Washington, DC: USEPA) 1982. Sunlight irradiations were performed on the samples of acrolein, the	

Section A7.1.1.1.2 Annex Point IIA7.1.1.1.2	Phototransformation in water including identity of transformation products	
	actinometer solution (10 µM p-nitroacetophenone/20 mM pyridine) and the controls, on consecutive cloudless days over a period of 4 to 8 days. Sampling occurred at 0, 18, 42, 66, and 90 hours. Photolyses were run at ambient temperature (25 ± 5 °C). During kinetic studies, acrolein was determined by HPLC and during product studies, it was analysed by direct UV spectrophotometry. The hydration product, 3-hydroxypropanal, was analysed by HPLC following derivatisation with PFPH.	
5.2 Results and discussion	The results show that photolysis is negligible compared to the dark hydration reaction. In addition, the run with 10 mg/l humic acid indicates that sensitised photolysis is unimportant. Because the hydration rate is unaffected by sunlight, the primary products must also be the same in light and dark. However, it is conceivable that the hydration product, 3-hydroxypropanal, is transformed photochemically. To test for this, product concentrations were determined as a function of time. This demonstrated that a material balance of reactant and product was obtained in both light and dark reactions.	
5.2.1 k^c_p		
5.2.2 K_{pE}	0.01 d^{-1}	
5.2.3 φ^c_E		
5.2.4 $t_{1/2E}$	70 days	
5.3 Conclusion	The photolysis of acrolein in water was found to proceed at a rate much slower than hydrolysis, and therefore the aqueous photolysis rate could not be measured. The maximum quantum yield was estimated to be ≤ 0.001. From this, the photolysis rate constant was calculated to be 0.01 d^{-1} and the minimum half-life was estimated to be 70 days under summer sunlight conditions at 40 °N. Since no photolysis occurred, no photolysis products could be found. However, it was shown that sunlight had no effect on the formation of the hydration product, 3-hydroxypropanal.	
5.3.1 Reliability	1	
5.3.2 Deficiencies	No	
	Evaluation by Competent Authorities	
	Use separate "evaluation boxes" to provide transparency as to the comments and views submitted	
	EVALUATION BY RAPPORTEUR MEMBER STATE	
Date	10/07/2007	
Materials and Methods	The Applicant's version is considered acceptable with the following exceptions: **2.3** No data on hours of daylight, see point **3.4.2.** **3.4.2 Table A7_1_1_1_2-2: Description of test system:** The hours of daylight have not been included in the table. This does not affect the endpoint from the study. **3.4.4 Temperature:** The stated temperature range is 25 ± 5°C. EPA guideline 161-2 states the desired range to be 25 ± 1°C. This does not affect the endpoint from the study.	

Section A7.1.1.1.2 **Annex Point IIA7.1.1.1.2**	**Phototransformation in water including identity of transformation products**	
Results and discussion	The Applicant’s version is considered to be acceptable	
Conclusion	The Applicant’s version is considered to be acceptable	
Reliability	1	
Acceptability	Acceptable	
Remarks	All endpoints and data presented in the summary have been checked against the original study and are correct.	
	COMMENTS FROM ... *(specify)*	
Date	*Give date of comments submitted*	
Materials and Methods	*Discuss additional relevant discrepancies referring to the (sub)heading numbers and to applicant's summary and conclusion.* *Discuss if deviating from view of rapporteur member state*	
Results and discussion	*Discuss if deviating from view of rapporteur member state*	
Conclusion	*Discuss if deviating from view of rapporteur member state*	
Reliability	*Discuss if deviating from view of rapporteur member state*	
Acceptability	*Discuss if deviating from view of rapporteur member state*	
Remarks		

Table A7_1_1_1_2-1: Description of test solution and controls

Criteria	Details
Purity of water	Unbuffered Milli-Q water
Preparation of test chemical solution	Solutions of 10 ppm acrolein in 10 mg/l humic acid prepared by diluting 0.5 ml of 1000 ppm acrolein stock, 5 ml of 100 mg/l humic acid stock and 1.0 ml of 0.5M pH 7 phosphate buffer to 50 ml.
Test concentrations (mg a.s./l)	Initial concentration: 10 ppm acrolein.
Temperature (°C)	Ambient 25°C ± 5°C
Preparation of a.s. solution	0.5 ml of p-nitroacetophenol stock and 161 µl of pyridine diluted to 100 ml with Milli-Q water.
Controls	None
Identity and concentration of co-solvent	No co-solvent used

Table A7_1_1_1_2-2: Description of test system

Criteria	Details
Laboratory equipment	Screw-capped 11 mm o.d. quartz tubes. HPLC: HP 1090 system Spectrometer: HP 8450 UV/Vis *Give details on the type and geometry of the reaction vessels (test tubes, material, size, type of absorption cell, pathlength); describe applicability in relationship to the applied wavelength.* *Report the name and the model of the spectrometer used.*
Test apparatus	*e.g. sunlight actinometer; describe details*
Properties of artificial light source:	No artificial light source used.
Properties of natural sunlight:	Natural sunlight used
Latitude	40ºN
Hours of daylight	Not stated
Time of year	Kinetic studies: 6 - 10 July 1987 Product studies: 26 May - 3 June 1988
Light intensity	Not stated
Solar irradiance (L_{λ})	Not stated

Table A7_1_1_1_2-3: Screening test results

Absorption curve	*give the plot of absorbanc of test substance vs. wavelenght (plus baseline)*
A_λ	*give the absorbance at wavelength λ for each replicate and the mean value.*
ε_λ^c	*give determined molar absorptivity (ε_λ^c) of the test substance (determined from absorption spectra*
k_{pEmax}	*give the calculated maximum direct aqueous photolysis sunlight rate constant $(K_{pE})_{max}$ for summer and winter solstices using appropriate L_λ values*
$t_{1/2Emin}$	*give the calculated minimum sunlight half-life in water bodies $(t_{1/2E})_{min}$*
L_λ	*Give the solar irradiance in water [10^{-3} einsteins cm^{-2} d^{-1}]*

Table A7_1_1_1_2-4: Actinometer data

PNAP/ pyridine concentrations	0.5l of PNAP stock and 161 µl of pyridine diluted to 100 ml with Milli-Q water *Give the molar concentration values of the actinometer chemicals at the start of each photolysis experiment and each time point t for each replicate (mean values).*
ϕ^a_E	3.4E-04 for 20 mM pyridine
k^a_p	*Give the rate constant for the used actinometer*

Table A7_1_1_1_2-5: Specification and amount of transformation products *(adjust table size as required)*

CAS-Number	***CAS and/or IUPAC* Chemical Name*(s)***	**Amount [%] of parent compound measured at**		
		pH_1	**pH_2**	**pH_3**

Section 7.1.1.2.1 Annex Point IIA VII.7.6.1.1		Ready Biodegradation	
		1 REFERENCE	Official use only
1.1	Reference	Tabak, H.H., Quave, S.A., Mashni, C.I., Barth, E.F., "Biodegradability studies with organic priority pollutant compounds", Journal WPCF, Volume 53, No. 10, Oct, 1981, pp1503-1518.	X
1.2	Data protection	No	
1.2.1	Data owner		
1.2.2	Criteria for data protection	Not applicable.	
		2 GUIDELINES AND QUALITY ASSURANCE	
2.1	Guideline study	Bunch, R.L. and Chambers, C.W., "A Biodegradability Test for Organic Compounds." Jour. Water Poll. Control Fed., 39, 181 (1967).	X
2.2	GLP	No	X
2.3	Deviations	Initial 7-day study, triplicate subcultures taken to 14 days. No information on the test substance. Specification of sewage sludge not given. Reference substance not the one specified by the guidelines. Results based on DOC and extraction from test substrate for detection by GC. Full range of controls not used.	
		3 METHOD	
3.1	Test material	Commercially available Acrolein.	
3.1.1	Lot/Batch number	Not stated.	X
3.1.2	Specification	Not stated.	X
3.1.3	Purity	Not stated.	X
3.1.4	Further relevant properties		
3.2	Reference substance	Yes, Phenol.	
3.2.1	Initial concentration of reference substance	5, 10 mg/l	
3.3	Testing procedure		
3.3.1	Test vessels	250 ml glass-stopped reagent bottles	
3.3.2	Test concentrations	5, 10 mg/l	
3.3.3	Controls	Blank control, inoculum – medium and substrate - medium control.	
3.3.4	Test conditions	The test with acrolein was carried out in glass-stopped reagent bottles to minimise volatilisation, inoculated with pre-chilled yeast extract and settled domestic wastewater. The bottles were incubated at a constant room temperature of 25°C in darkness.	X

Section 7.1.1.2.1 Annex Point IIA VII.7.6.1.1		Ready Biodegradation	
3.3.5	Duration of test	28 days	
3.3.6	Analytical parameters		
3.3.7	Sampling	Duplicate samples at the beginning of each incubation period and triplicate samples at the end of the 7 day incubation	
3.3.8	Analysis of study data		
		4 RESULTS	
4.1	Ready Biodegradability	The seven day culture (and all of the further subcultures) showed 100% biodegradation at both initial concentrations of 5 and 10 mg/l.	
4.2	Dissolved Oxygen		
		5 APPLICANT'S SUMMARY AND CONCLUSION	
5.1	**Materials and methods**	The biodegradability test method used was the static-culture flask-screening procedure of Bunch and Chambers, utilising biochemical oxygen demand (BOD) dilution water containing 5 mg yeast extract per litre, as the synthetic medium; 5 and 10 mg/l concentrations of the test compound, a 7 day static incubation of 25°C in the dark, followed by three weekly subcultures, incorporating settled domestic wastewater as microbial inoculum. The test was modified to include the capability to study volatile compounds and to facilitate the use of GC, DOC and TOC analytical procedures. The procedure was extended to include the determination of the initial concentration of the test compound at the beginning of each incubation period. Aqueous stock solutions were used to prepare the culture media. Biodegradability studies with acrolein were carried out in glass-stopped reagent bottles to minimise volatilisation. These were then inoculated with the pre-chilled yeast extract and settled domestic wastewater inoculum, before incubation at a constant room temperature of 25°C in darkness. Duplicate samples at the beginning of each incubation period and triplicate samples at the end of the 7 day incubation were subjected to GC and DOC analysis as follows: The culture samples were extracted three times with 20 ml portions of methylene chloride. The pooled solvent extracts were evaporated by the Kuderna-Danish evaporation technique and the concentrated extracts were then processed for GC analysis. For DOC, the samples were membrane filtered through a system using 0.22 μm porosity filters.	
5.2	**Results and discussion**	The seven-day culture (and all of the further subcultures) showed 100% biodegradation at both initial concentrations of 5 and 10 mg/l. The 100% biodegradation results only indicate that test substance concentrations had fallen below the detectable level. The minimum sensitivity of the GC procedures used was about 0.1 mg/l, as the procedure was not optimised for sensitivity. The extraction efficiency differed with each of the test compounds and the recovery value ranged from 78 to 98% and were fairly reproducible for several test runs with each of the substrate-dosed culture samples.	X
5.3	**Conclusion**	Acrolein was shown to be easily dissimilated with rapid acclimation of microbiota to the substrate.	X

Section 7.1.1.2.1 Annex Point IIA VII.7.6.1.1	Ready Biodegradation	
	The reliability of 2 was given in the EU risk assessment of Acrolein.	
5.3.1 Reliability	2	
5.3.2 Deficiencies	Not to standard test guideline.	
	Evaluation by Competent Authorities	
	Use separate "evaluation boxes" to provide transparency as to the comments and views submitted	
	EVALUATION BY RAPPORTEUR MEMBER STATE	
Date	21/03/2006	
Materials and Methods	The Applicant's version is considered to be acceptable, noting the following: **1.1** The data submitted is taken from a published study and no raw data or quality assurance statement is given. **2.1** A copy of the guideline 'Bunch, R.L. and Chambers, C.W., "A Biodegradability Test for Organic Compounds." Jour. Water Poll. Control Fed. 39, 181 (1967)' was not accessible, therefore the evaluation by the UK CA is carried out using a scientific comparison with the available OECD guidelines. **2.2** As the study was published before 1989, it is exempt from GLP. **3.1.1** Batch number not stated. **3.1.2** Specification not stated. **3.1.3** Purity not stated. **3.3.4** Test carried out at 25°C, OECD guidelines state test to be carried out at 30°C.	
Results and discussion	The Applicant's version is considered to be acceptable, noting the following: **5.2** No tabulated results are presented in the RSS, however the following results are available in the original paper: Table 5: Biodegradability of Acrolein. (see table below) D*= significant degradation with rapid adaptation.	
Conclusion	The Applicant's version is considered to be acceptable, noting the following: **5.3** The statement '*Acrolein was shown to be easily dissimilated with rapid acclimation of microbiota to the substrate*' is a statement by the author of the original paper. There are no data presented to support this.	
Reliability	3	
Acceptability	Not Acceptable. The reliability level has been changed from a 2 to a 3 because the UK CA believes that there are a number of deficiencies in the methodology and reporting of the original study.	

Table 5: Biodegradability of Acrolein.

Test Compound	Conc. Of test Compound (mg/L)	Performance summary	Average of 3 test flasks (Biodegradation of test compound in 7 days (%))			
			Original Culture	1st Culture	2nd Culture	3rd culture
Acrolein	5	D*	100	100	100	100
Acrolein	10	D*	100	100	100	100

D*= significant degradation with rapid adaptation.

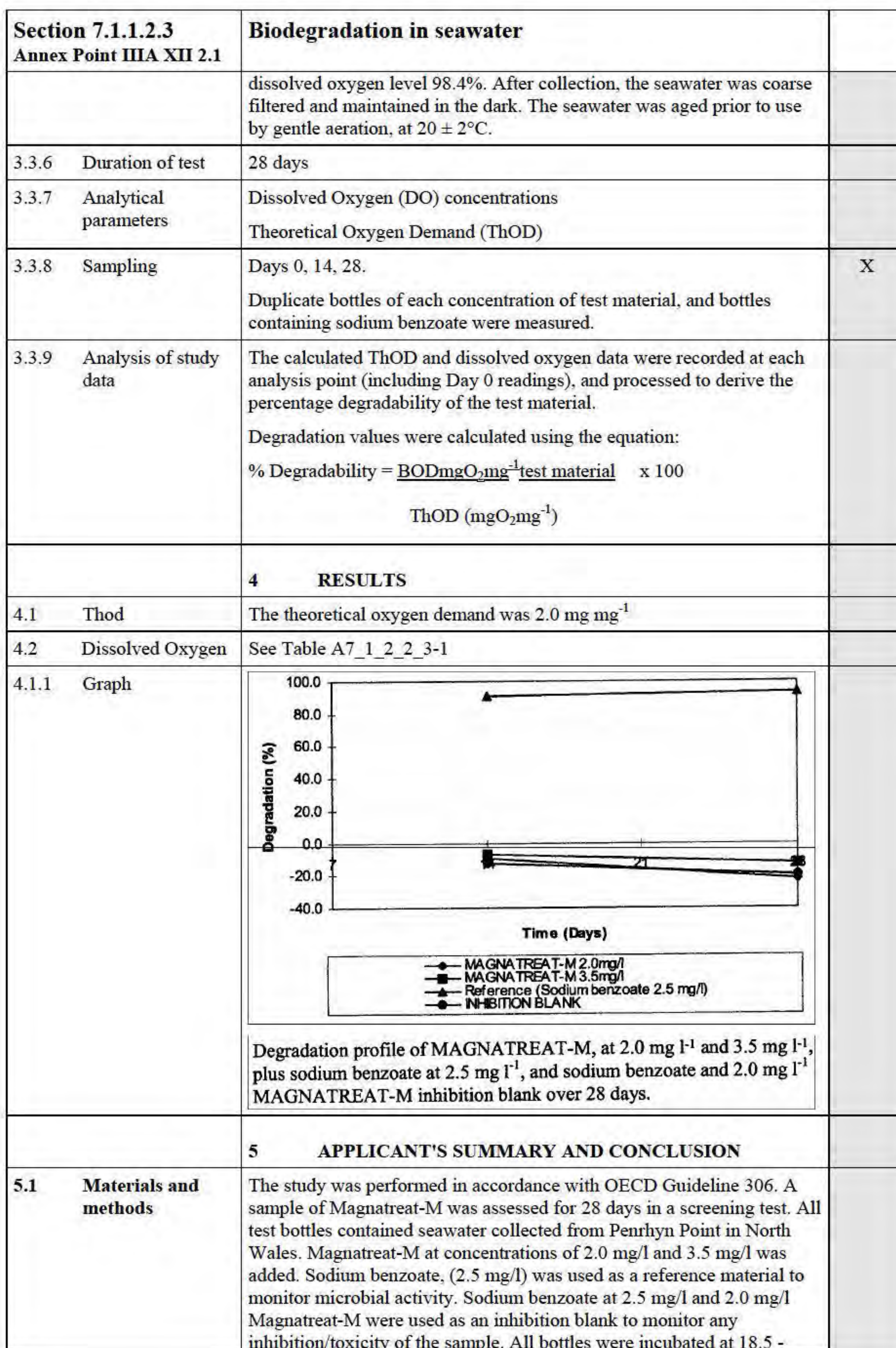
Section 7.1.1.2.1 **Annex Point IIA VII.7.6.1.1**	**Ready Biodegradation**	
Remarks	The guideline 'Bunch, R.L. and Chambers, C.W., 'A Biodegradability Test for Organic Compounds." Jour. Water Poll. Control Fed. 39, 181 (1967)', was not available to view and therefore the reliability level was changed as an accurate evaluation could not be made. [This has been requested so the remark may change]. As no tabulated results or graphs were included in the RSS, the reporting was considered to be deficient. All endpoints addressed in the summary have been checked against those in the study. Taking the above factors into account, the UK CA considers that this study can only be used as supporting evidence that acrolein would degrade in the aquatic environment.	
	COMMENTS FROM ... *(specify)*	
Date	*Give date of comments submitted*	
Materials and Methods	*Discuss additional relevant discrepancies referring to the (sub)heading numbers and to applicant's summary and conclusion.* *Discuss if deviating from view of rapporteur member state*	
Results and discussion	*Discuss if deviating from view of rapporteur member state*	
Conclusion	*Discuss if deviating from view of rapporteur member state*	
Reliability	*Discuss if deviating from view of rapporteur member state*	
Acceptability	*Discuss if deviating from view of rapporteur member state*	
Remarks		

Section A7.1.1.2.2 Annex Point IIA VII.7.6.1.2	Inherent biodegradability	
	JUSTIFICATION FOR NON-SUBMISSION OF DATA	**Official use only**
Other existing data [ ]	**Technically not feasible [ ]** **Scientifically unjustified [X]**	
Limited exposure [ ]	**Other justification [ ]**	
Detailed justification:	As a ready biodegradability study was carried out and gave a positive result (Section A7.1.1.2.1, Annex Point IIA, VII.7.6.1.2.), in accordance with the TNsG on Data Requirements for the Biocidal Products Directive an inherent biodegradability study is not required. In addition the active substance has been shown to undergo rapid degradation by physico-chemical processes including rapid volatilisation (A7.2.1) and photodegradation (A7.1.1.1.2). and microbial degradation in water (anaerobic and aerobic freshwater-sediment radio-labelled studies, A7.1.2.1.1 and A7.1.2.1.2) transforming the active substance to CO2.	
Undertaking of intended data submission [ ]		
	Evaluation by Competent Authorities	
	Use separate "evaluation boxes" to provide transparency as to the comments and views submitted	
	EVALUATION BY RAPPORTEUR MEMBER STATE	
Date	30/11/2007	
Evaluation of applicant's justification	The UK CA has made the decision at the evaluation stage that the ready biodegradation test is not acceptable as a stand alone endpoint. However, due to the exposure route i.e. not via an STP, and the availability of other data to show degradation no additional data are considered necessary for this specific use pattern.	
Conclusion	Acceptable because of the availability of other studies and not on the basis of the ready biodegradability.	
Remarks		
	COMMENTS FROM OTHER MEMBER STATE *(specify)*	
Date	*Give date of comments submitted*	
Evaluation of applicant's justification	*Discuss if deviating from view of rapporteur member state*	
Conclusion	*Discuss if deviating from view of rapporteur member state*	
Remarks		

Section A7.1.1.2.2 Annex Point IIA VII.7.6.1.2	Inherent biodegradability	
	JUSTIFICATION FOR NON-SUBMISSION OF DATA	Official use only
Other existing data [ ]	**Technically not feasible [ ]** **Scientifically unjustified [X]**	
Limited exposure [ ]	**Other justification [ ]**	
Detailed justification:	As a ready biodegradability study was carried out and gave a positive result (Section A7.1.1.2.1, Annex Point IIA, VII.7.6.1.2.), in accordance with the TNsG on Data Requirements for the Biocidal Products Directive an inherent biodegradability study is not required. In addition the active substance has been shown to undergo rapid degradation by physico-chemical processes including rapid volatilisation (A7.2.1) and photodegradation (A7.1.1.1.2). and microbial degradation in water (anaerobic and aerobic freshwater-sediment radio-labelled studies, A7.1.2.1.1 and A7.1.2.1.2) transforming the active substance to CO2.	
Undertaking of intended data submission [ ]		
	Evaluation by Competent Authorities	
	Use separate "evaluation boxes" to provide transparency as to the comments and views submitted	
	EVALUATION BY RAPPORTEUR MEMBER STATE	
Date	30/11/2007	
Evaluation of applicant's justification	The UK CA has made the decision at the evaluation stage that the ready biodegradation test is not acceptable as a stand alone endpoint. However, due to the exposure route i.e. not via an STP, and the availability of other data to show degradation no additional data are considered necessary for this specific use pattern.	
Conclusion	Acceptable because of the availability of other studies and not on the basis of the ready biodegradability.	
Remarks		
	COMMENTS FROM OTHER MEMBER STATE *(specify)*	
Date	*Give date of comments submitted*	
Evaluation of applicant's justification	*Discuss if deviating from view of rapporteur member state*	
Conclusion	*Discuss if deviating from view of rapporteur member state*	
Remarks		

Section A7.1.1.2.2 **Annex Point IIA** **VII.7.6.1.2**	**Inherent biodegradability**	
Section A7.1.1.2.2 **Annex Point IIA** **VII.7.6.1.2**	**Inherent biodegradability**	
	JUSTIFICATION FOR NON-SUBMISSION OF DATA	**Official use only**
Other existing data [ ] **Limited exposure [ ]**	**Technically not feasible [ ]** **Scientifically unjustified [X]** **Other justification [ ]**	
Detailed justification:	As a ready biodegradability study was carried out and gave a positive result (Section A7.1.1.2.1, Annex Point IIA, VII.7.6.1.2.), in accordance with the TNsG on Data Requirements for the Biocidal Products Directive an inherent biodegradability study is not required. In addition the active substance has been shown to undergo rapid degradation by physico-chemical processes including rapid volatilisation (A7.2.1) and photodegradation (A7.1.1.1.2). and microbial degradation in water (anaerobic and aerobic freshwater-sediment radio-labelled studies, A7.1.2.1.1 and A7.1.2.1.2) transforming the active substance to CO2.	
Undertaking of intended data submission [ ]		
	Evaluation by Competent Authorities	
	Use separate "evaluation boxes" to provide transparency as to the comments and views submitted	
	EVALUATION BY RAPPORTEUR MEMBER STATE	
Date	*Give date of action*	
Evaluation of applicant's justification	*Discuss applicant's justification and, if applicable, deviating view*	
Conclusion	*Indicate whether applicant's justification is acceptable or not. If unacceptable because of the reasons discussed above, indicate which action will be required, e.g. submission of specific test/study data*	
Remarks		
	COMMENTS FROM OTHER MEMBER STATE *(specify)*	
Date	*Give date of comments submitted*	
Evaluation of applicant's justification	*Discuss if deviating from view of rapporteur member state*	
Conclusion	*Discuss if deviating from view of rapporteur member state*	
Remarks		

Section 7.1.1.2.3 Annex Point IIIA XII 2.1		Biodegradation in seawater	
		1 REFERENCE	**Official use only**
1.1	**Reference**	Manley, R. (2003a) A Study of the Aerobic Biodegradation in Seawater of MAGNATREAT-M using the Closed Bottle Procedure in a Screening Test. Severn Trent Limited. Study No. STL031989.	
1.2	**Data protection**	Yes	
1.2.1	Data owner	Baker Petrolite	
1.2.2	Criteria for data protection	Data on new a.s. for first entry to Annex I	
		2 GUIDELINES AND QUALITY ASSURANCE	
2.1	**Guideline study**	Yes OECD Guideline 306	
2.2	**GLP**	Yes	
2.3	**Deviations**	No	X
		3 METHOD	
3.1	**Test material**	Magnatreat M: As given in Section 2	X
3.1.1	Lot/Batch number	STL reference: 832111	
3.1.2	Specification	As given in Section 2	X
3.1.3	Purity	Not stated	
3.1.4	Further relevant properties	None	
3.2	**Reference substance**	Yes	
3.2.1	Initial concentration of reference substance	Sodium benzoate: 2.5mg/l	
3.3	**Testing procedure**		
3.3.1	Test vessels	Completely filled, sealed glass biological oxygen demand (BOD) bottles of nominal 272 ml volume.	
3.3.2	Test concentrations	Magnatreat-M used at 2.0 mg/l and 3.5 mg/l. Soluble test materials are added to the test media from a 1.0 g/l stock solution	
3.3.3	Controls	Sodium benzoate, at a concentration of 2.5 mg/l was used to as a reference substance to monitor microbial activity. Sodium benzoate at 2.5 mg/l and 2.0 mg/l Magnatreat-M were used as an inhibition blank to monitor any inhibition/toxicity of the sample.	
3.3.4	Test conditions	All test bottles contained coarse filtered, natural seawater as inoculum. For each of the sample days, duplicate bottles were prepared for each of the test material concentrations and sodium benzoate. All bottles were incubated at 18.5 - 21.0°C in the dark. The incubator was at 21°C for one day only and was adjusted back to 15.0-20.0°C.	
3.3.5	Source of seawater	Natural seawater was collected from Penrhyn Point in North Wales. The temperature at collection was 9.5°C, pH 7.96, salinity 32.9 g/l and the	X



Section 7.1.1.2.3 **Annex Point IIIA XII 2.1**		**Biodegradation in seawater**	
		dissolved oxygen level 98.4%. After collection, the seawater was coarse filtered and maintained in the dark. The seawater was aged prior to use by gentle aeration, at 20 ± 2°C.	
3.3.6	Duration of test	28 days	
3.3.7	Analytical parameters	Dissolved Oxygen (DO) concentrations Theoretical Oxygen Demand (ThOD)	
3.3.8	Sampling	Days 0, 14, 28. Duplicate bottles of each concentration of test material, and bottles containing sodium benzoate were measured.	X
3.3.9	Analysis of study data	The calculated ThOD and dissolved oxygen data were recorded at each analysis point (including Day 0 readings), and processed to derive the percentage degradability of the test material. Degradation values were calculated using the equation: $\% \text{ Degradability} = \frac{\text{BOD} mgO_2mg^{-1} \text{test material}}{\text{ThOD } (mgO_2mg^{-1})} \times 100$	
		4 RESULTS	
4.1	Thod	The theoretical oxygen demand was 2.0 mg mg^{-1}	
4.2	Dissolved Oxygen	See Table A7_1_2_2_3-1	
4.1.1	Graph	Degradation (%) 100.0 80.0 60.0 40.0 20.0 0.0 -20.0 -40.0 7 21 28 Time (Days) MAGNATREAT-M 2.0mg/l MAGNATREAT-M 3.5mg/l Reference (Sodium benzoate 2.5 mg/l) INHIBITION BLANK Degradation profile of MAGNATREAT-M, at 2.0 mg l^{-1} and 3.5 mg l^{-1}, plus sodium benzoate at 2.5 mg l^{-1}, and sodium benzoate and 2.0 mg l^{-1} MAGNATREAT-M inhibition blank over 28 days.	
		5 APPLICANT'S SUMMARY AND CONCLUSION	
5.1	**Materials and methods**	The study was performed in accordance with OECD Guideline 306. A sample of Magnatreat-M was assessed for 28 days in a screening test. All test bottles contained seawater collected from Penrhyn Point in North Wales. Magnatreat-M at concentrations of 2.0 mg/l and 3.5 mg/l was added. Sodium benzoate, (2.5 mg/l) was used as a reference material to monitor microbial activity. Sodium benzoate at 2.5 mg/l and 2.0 mg/l Magnatreat-M were used as an inhibition blank to monitor any inhibition/toxicity of the sample. All bottles were incubated at 18.5 -	

Section 7.1.1.2.3 Annex Point IIIA XII 2.1	Biodegradation in seawater	
	21°C in the dark for 28 days. Dissolved oxygen and theoretical oxygen demand were measured on Days 0, 14 and 28.	
5.2 Results and discussion	A figure of 60% degradation within 28 days is usually taken as being indicative of a good potential for degradation in the marine environment. Under the test condition in the closed bottle procedure, Magnatreat-M showed limited potential for degradation in the marine environment at test concentrations of 2.0 and 3.5 mg/l. It was concluded from the inclusion of an inhibition blank that the sample was either toxic or inhibitive to the micro-organisms present. **% Degradability** Material (mg/l): Magnatreat M Day 14: Negative value, indicating possible toxicity/inhibition. Day 28: Negative value, indicating possible toxicity/inhibition. Material (mg/l): Magnatreat-M (3.5) Day 14: Negative value, indicating possible toxicity/inhibition. Day 28: Negative value, indicating possible toxicity/inhibition. Material (mg/l): Sodium benzoate (2.5)* Day 14: 91.3 % Day 28: 93.9 % Material (mg/l): Inhibition blank, Sodium benzoate (2.5) + Magnatreat-M at (2.0) Day 14: Negative value, indicating possible toxicity/inhibition. Day 28: Negative value, indicating possible toxicity/inhibition. *Using the calculated theoretical oxygen demand (ThOD) of sodium benzoate as 1.67 mg O_2/l A degradation of 93.9% after 28 days was obtained from sodium benzoate. This demonstrates that the inoculum was biologically active. Negative values indicated inhibition or toxicity by the test material.	X
5.3 Conclusion		X
5.3.1 Reliability	1	
5.3.2 Deficiencies	No.	X

Section 7.1.1.2.3 Annex Point IIIA XII 2.1	Biodegradation in seawater	
	Evaluation by Competent Authorities	
	Use separate "evaluation boxes" to provide transparency as to the comments and views submitted	

	EVALUATION BY RAPPORTEUR MEMBER STATE
Date	24/03/2006
Materials and Methods	The Applicant's version is acceptable, noting the following: **2.3** Deviations were made, see points **3.1, 3.1.2, 3.3.5** and **3.3.8** below. **3.1, & 3.1.2** No details provided in the study, or the summary, on the test substance 'MAGNATREAT-M' to compare with details in section 2. 'Section 2' refers to section 2 of Doc III, but there is nothing in the report to verify this. **3.3.5** Information on the seawater missing from the original study. Namely, depth of collection, appearance of seawater, length of time between collection and use, and the length of time the seawater was aged prior to use. **3.3.8** OECD guideline 306 that states analysis should be performed after 5, 15 and 28 days as a minimum.
Results and discussion	The Applicant's version is considered to be acceptable, noting the following; **5.2** The first % degradability summary does not state the concentration of MAGNATREAT-M in the test solution. This should read MAGNATREAT-M (2.0)
Conclusion	The Applicant's version is considered to be acceptable, noting the following; **5.3** No conclusion provided by the Applicant. The UK CA suggests the following should be used; 'It was concluded from the inclusion of an inhibition blank that the sample was either toxic or inhibitory to the microorganisms present in the seawater. A degradation of 93.9% after 28 days was obtained from sodium benzoate demonstrating that the inoculum was biologically active'. Further testing, using a lower concentration of test substance, may address this issue. However, the toxicity of acrolein is such that derivation of a valid (measured) endpoint would be unlikely.
Reliability	2
Acceptability	Acceptable **5.3.2** The reliability level has been changed from a 1 to a 2 because the UK CA believes that there are a number of deficiencies in the methodology and reporting.
Remarks	The UK CA believes that the study was performed correctly with only minor deviations from OECD guideline 306. All endpoints addressed in the summary have been checked against those in the study. Under the conditions tested Acrolein has not been shown to be readily biodegradable in seawater. This study should have been performed with lower test concentrations.
	COMMENTS FROM ... *(specify)*
Date	*Give date of comments submitted*

Section 7.1.1.2.3 **Annex Point IIIA XII 2.1**	**Biodegradation in seawater**	
Materials and Methods	*Discuss additional relevant discrepancies referring to the (sub)heading numbers and to applicant's summary and conclusion.* *Discuss if deviating from view of rapporteur member state*	
Results and discussion	*Discuss if deviating from view of rapporteur member state*	
Conclusion	*Discuss if deviating from view of rapporteur member state*	
Reliability	*Discuss if deviating from view of rapporteur member state*	
Acceptability	*Discuss if deviating from view of rapporteur member state*	
Remarks		

Table A7_1_2_2_3-1: Dissolved oxygen (mg/l) data for control and inoculum blanks and test media containing MAGNATREAT-M

Culture medium	Flask No.	mg O_2/l after n days		
		Day 0	Day 14	Day 28
Test: Nutrient fortified seawater with 2.0 mg/l test material	1	7.65	7.15	7.07
	2	7.66	7.15	7.07
	Mean	7.65	7.15	7.07
Test: Nutrient fortified seawater with 3.5 mg/l test material	1	7.66	7.25	7.09
	2	7.71	7.30	7.10
	Mean	7.69	7.28	7.10
Reference: Nutrient fortified seawater with 2.5 mg/l sodium benzoate	1	7.64	3.00	2.10
	2	7.66	2.92	2.40
	Mean	7.65	2.96	2.25
Blank: Nutrient fortified seawater only	1	7.62	6.80	6.16
	2	7.64	6.70	6.14
	Mean	7.63	6.75	6.15
Reference: Nutrient fortified seawater with 2.5 mg/l sodium benzoate and 2.0 mg/l test material	1	7.62	7.30	6.92
	2	7.63	7.21	7.03
	Mean	7.63	7.26	6.98

Section A7.1.2 **Annex Point IIIA XII.2.1**	**Rate and route of degradation in aquatic systems including identification of metabolites and degradation products**	
	JUSTIFICATION FOR NON-SUBMISSION OF DATA	**Official use only**
Other existing data [ ] **Limited exposure [ ]**	**Technically not feasible [ ]** **Scientifically unjustified [X]** **Other justification [ ]**	
Detailed justification:	The rate and route of degradation in water/sediment has been determined and discussed in section IIIA7.1.2.1.1 & IIIA7.1.2.1.2	
Undertaking of intended data submission [ ]		
	Evaluation by Competent Authorities	
	Use separate "evaluation boxes" to provide transparency as to the comments and views submitted	
	EVALUATION BY RAPPORTEUR MEMBER STATE	
Date	18/05/2006	
Evaluation of applicant's justification	The Applicant's justification is acceptable.	
Conclusion	Acceptable	
Remarks		
	COMMENTS FROM OTHER MEMBER STATE *(specify)*	
Date	*Give date of comments submitted*	
Evaluation of applicant's justification	*Discuss if deviating from view of rapporteur member state*	
Conclusion	*Discuss if deviating from view of rapporteur member state*	
Remarks		

Section A7.1.2.1.1 **Annex Point IIIA XII.2.1**	**Biological sewage treatment: Aerobic simulation study**	
	JUSTIFICATION FOR NON-SUBMISSION OF DATA	**Official use only**
Other existing data [ ]	**Technically not feasible [ ]** **Scientifically unjustified [X]**	
Limited exposure [ ]	**Other justification [ ]**	
Detailed justification:	The active substance will not be released to biological sewage treatment plants before release as it is used exclusively in the marine environment on off-shore oil product platforms. An aerobic simulation study is therefore considered to be scientifically unjustified.	
Undertaking of intended data submission [ ]		
	Evaluation by Competent Authorities	
	Use separate "evaluation boxes" to provide transparency as to the comments and views submitted	
	EVALUATION BY RAPPORTEUR MEMBER STATE	
Date	16/05/2006	
Evaluation of applicant's justification	The Applicant's justification is acceptable	
Conclusion	Acceptable	
Remarks		
	COMMENTS FROM OTHER MEMBER STATE *(specify)*	
Date	*Give date of comments submitted*	
Evaluation of applicant's justification	*Discuss if deviating from view of rapporteur member state*	
Conclusion	*Discuss if deviating from view of rapporteur member state*	
Remarks		

Section A7.1.2.1.2 **Annex Point IIIA XII.2.1**	**Biological sewage treatment: anaerobic degradation study**	
	JUSTIFICATION FOR NON-SUBMISSION OF DATA	**Official use only**
Other existing data [ ] **Limited exposure [ ]**	**Technically not feasible [ ]** **Scientifically unjustified [ ]** **Other justification [ ]**	
Detailed justification:	The active substance will not be released to biological sewage treatment plants before release as it is used exclusively in the marine environment on off-shore oil product platforms. An anaerobic degradation study is therefore considered to be scientifically unjustified.	
Undertaking of intended data submission [ ]		
	Evaluation by Competent Authorities	
	Use separate "evaluation boxes" to provide transparency as to the comments and views submitted	
	EVALUATION BY RAPPORTEUR MEMBER STATE	
Date	16/05/2006	
Evaluation of applicant's justification	The Applicant's justification is acceptable.	
Conclusion	Acceptable	
Remarks		
	COMMENTS FROM OTHER MEMBER STATE *(specify)*	
Date	*Give date of comments submitted*	
Evaluation of applicant's justification	*Discuss if deviating from view of rapporteur member state*	
Conclusion	*Discuss if deviating from view of rapporteur member state*	
Remarks		

Section 7.1.2.2.1 Annex Point IIIA XII 2.1		Aerobic aquatic degradation	
		1 REFERENCE	Official use only
1.1	**Reference**	Smith, A.M. (1993a). (^{14}C-Acrolein) - Determination of the Aerobic Aquatic Metabolism, Springborn Laboratories, Inc. SLI Report No. 91-3-3747.	
1.2	**Data protection**	Yes	
1.2.1	Data owner	Baker Petrolite	
1.2.2	Criteria for data protection	Data on new a.s. for first entry to Annex I	
		2 GUIDELINES AND QUALITY ASSURANCE	
2.1	**Guideline study**	Yes US EPA FIFRA Guideline 162-4	
2.2	**GLP**	Yes	
2.3	**Deviations**	No	
		3 METHOD	
3.1	**Test material**	As given in Section 2	
3.1.1	Lot/Batch number	Sample no. 6587	X
3.1.2	Specification	As given in Section 2	
3.1.3	Purity	95.06%	X
3.1.4	Further relevant properties	Acrolein has a water solubility of 23.7% at 25°C.	
3.1.5	Composition of Product	Not applicable	
3.1.6	TS inhibitory to microorganisms	Yes Exposure to increasing concentrations of acrolein had increasingly inhibitory effects upon the population of *Anabaena flos-aquae.* The effects of test substance on mean standing crop on day 5, relative to control, ranged from 5.12% to 98.6% inhibition.	
3.1.7	Specific chemical analysis	None used	
3.2	**Reference substance**	No	
3.2.1	Initial concentration of reference substance		
3.3	**Testing procedure**		
3.3.1	Inoculum / test species	See Table A7_1_2_1_2-1	
3.3.2	Test system	See Table A7_1_2_1_2-2	
3.3.3	Test conditions	See Table A7_1_2_1_2-3	X

Section 7.1.2.2.1 Annex Point IIIA XII 2.1		Aerobic aquatic degradation	
3.3.4	Method of preparation of test solution	A radiolabelled superstock solution was prepared by quantitatively transferring the entire contents of an ampoule of radiolabelled ^{14}C-Acrolein (100 mCi) through repetitive rinsing with Burdick and Jackson high purity acetone into a 100 ml volumetric flask and diluting to volume. This super-stock had a mean measured concentration of 4.30 mg/ml (triplicate analysis by liquid scintillation counting (LSC)). A 1.25 ml sample of the 4.30 mg/ml radiolabelled stock was combined with 32.125 mg of non-radiolabelled acrolein and diluted to a final volume of 25 ml with NANOpure® water, to obtain a dosing solution concentration of 1.50 mg/ml acrolein. Exactly 4.00 ml of this solution was added by gas-tight syringe to each replicate test vessel containing sediment and 400 ml of canal water to obtain a nominal concentration of 15.0 mg/l.	
3.3.5	Initial TS concentration	15.0 mg/l	
3.3.6	Duration of test	32 days	X
3.3.7	Analytical parameter	Rate of metabolism and pattern of decline of ^{14}C-acrolein.	
3.3.8	Sampling	The sampling intervals for this study were chosen as events where maximum levels of each degradation product would be expected based on the results observed in the interim study. Sediment samples were taken for microbial biomass determinations at initiation and termination of the study. At hours 0, 3, and 5 and Days 1, 2, 5 and 32, HPLC and LSC analysis samples were drawn. On Day 32 the canal water was decanted and the volume recorded. Percent moisture analysis and radiometric combustion analysis was carried out on the remaining sediment. Sub-samples were extracted with 120 ml of sodium hydroxide and analysed by HPLC and LSC techniques. After extraction, radiometric combustion samples were weighed and analysed for non-extractable residues. The sodium hydroxide trapping systems were replaced and analysed at each sampling interval except Hour 0. In order to preclude saturation, additional trap changes were performed on Days 3, 4, 6, 7, 8, 9, 11, 12, 14, 17, 20 and 25 over the 32-day study. The total volume of the sodium hydroxide traps was measured and samples were analysed by LSC. At Day 32, the Tenax® traps were eluted twice sequentially with methanol and the eluent analysed by LSC. Representative sodium hydroxide traps (replicate 1 Day 3, 11, 25, and 32 and replicate 3 Day 25) were analysed by barium hydroxide precipitation procedure to determine the presence of ^{14}C-carbon dioxide Replicate 1 Day 32 canal water was also analysed to confirm the presence of ^{14}C-carbon dioxide Samples were treated with a saturated barium hydroxide solution and the resulting precipitate filtered. Precipitate and supernatant liquid were subsequently analysed by LSC.	
3.3.9	Intermediates/ degradation products	Identified High performance liquid chromatography with radiometric detection (HPLC-RAM) of the natural water phase collected at Hours 0, 3 and 5 and on Days 1, 2, 5 and 32, revealed the rapid degradation of ^{14}C-acrolein. Through Day 5 of the study, six products were produced in the water phase which were ephemeral in nature: 3-hydroxypropanal, acrylic acid, allyl alcohol, propionic acid, glyceric acid and 3-hydropropionic acid. An additional product, oxalic acid, was formed on Day 2 and	

Section 7.1.2.2.1 Annex Point IIIA XII 2.1	Aerobic aquatic degradation	
	remained throughout the study. All of these metabolites were further mineralised to carbon dioxide.	
3.3.10 Controls	Not specified	X
3.3.11 Statistics	The rate constant and half-life of acrolein in natural water under aerobic aquatic conditions were determined in this study. The interim study presents rate constants and half-lives in both the canal water and sediment phases. A cumulative material balance was calculated for each replicate at each sampling interval and a final material balance was calculated upon termination. The final material balance was calculated by summing the cumulative disintegrations per minute (DPM) recovered in the carbon dioxide and Tenax® traps, DPM recovered in the canal water, DPM recovered in the sediment extract, and the non-extractable DPM remaining in the sediment, and then dividing by the total DPM applied in the dose.	
	4 RESULTS	
4.1 Degradation of test substance		
4.1.1 Degradation of TS in abiotic control	Not specified	
4.1.2 Degradation	Carbon dioxide, the primary degradation product was formed in the water phase on Day 2 and remained throughout the study. Expressed as bicarbonate ion (HCO_3^-), carbon dioxide represented greater than 90% of the HPLC-RAM peak area on Days 5 and 32 and was observed to be 40% (4.7 ppm acrolein equivalents) and 25% (2.9 ppm acrolein equivalents) of the initial dose on the Day 5 and Day 32 sampling events, respectively.	
4.1.3 Graph		

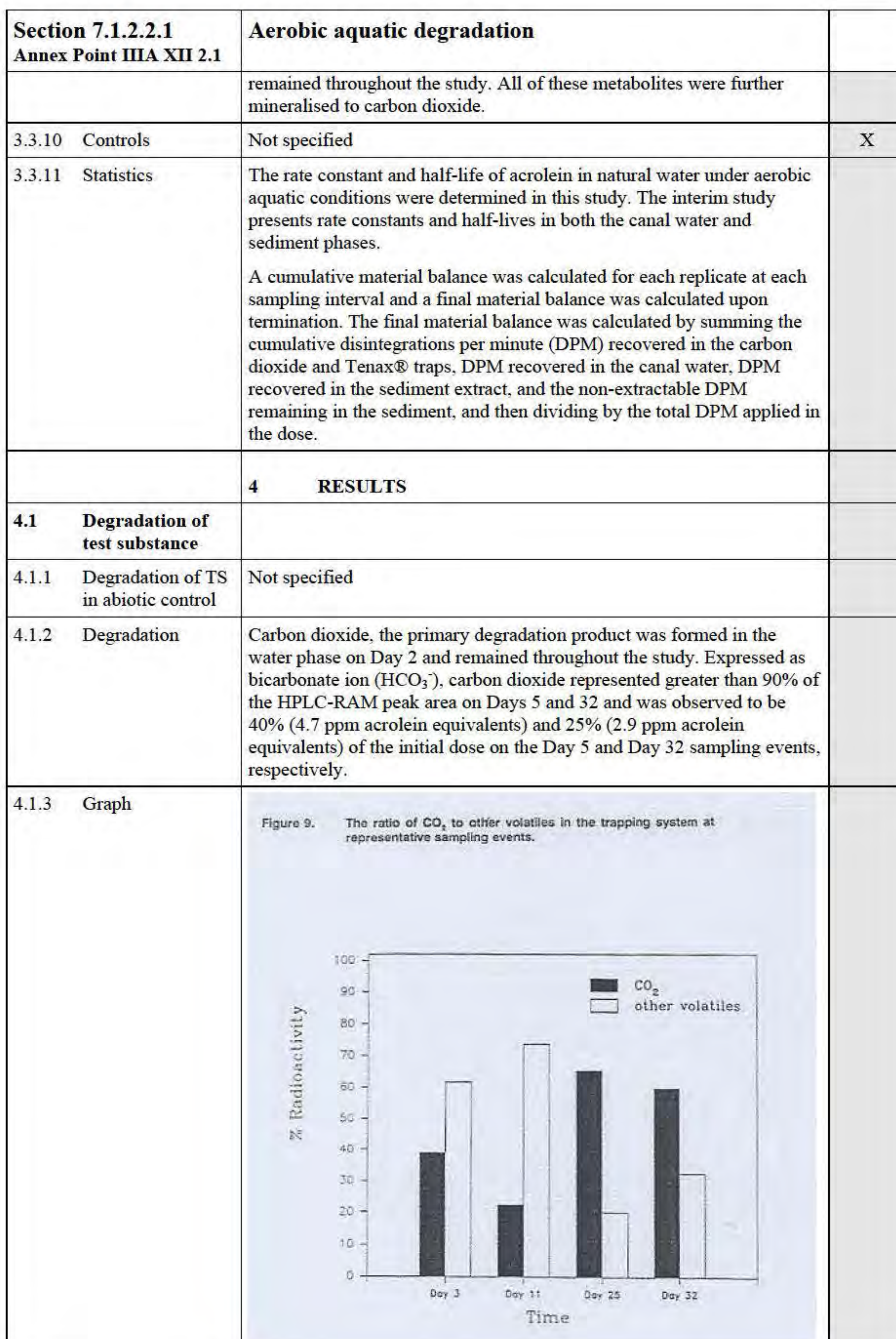


Figure 9. The ratio of CO_2 to other volatiles in the trapping system at representative sampling events.

Section 7.1.2.2.1 Annex Point IIIA XII 2.1	Aerobic aquatic degradation	
	Figure 1: **The Ratio of Carbon-dioxide to Other Volatiles in the Trapping System at Representative Sampling Events**	
4.1.4 Other observations	None	
4.1.5 Degradation of reference substance	Not applicable	
4.1.6 Intermediates/ degradation products	See Section 5.2	
	5 APPLICANT'S SUMMARY AND CONCLUSION	
5.1 Materials and methods	US EPA FIFRA Guideline No. 162-4	
5.2 Results and discussion	HPLC results of canal water samples as percent of peak area	X

HPLC results of canal water samples as percent of peak area

	Acrolein	3-hydroxy propanal	acrylic acid	allyl alcohol	propionic acid	oxalic acid	3-hydroxy propionic acid	sum	bi-carb-onate	glyceris acid
Hour 0										
R1	78	6	10	6	ND	ND	ND	ND	ND	ND
R2	76	5	11	8	ND	ND	ND	ND	ND	ND
R3	74	4	7	10	ND	ND	ND	ND	ND	ND
Hour 3										
R1	76	5	12	7	ND	ND	ND	ND	ND	ND
R2	76	5	13	6	ND	ND	ND	ND	ND	ND
R3	72	7	12	8	ND	ND	ND	ND	ND	ND
Hour 5										
R1	72	7	12	6	ND	ND	ND	ND	ND	ND
R2	71	10	13	6	ND	ND	ND	ND	ND	ND
R3	69	8	13	10	ND	ND	ND	ND	ND	ND
Day 1										
R1	55	24	14	6	ND	ND	ND	ND	ND	ND
R2	53	25	15	7	ND	ND	ND	ND	ND	ND
R3	52	23	20	5	ND	ND	ND	ND	ND	ND
Day 2										
R1	ND	12	23	4	22	2	17	65	12	ND
R2	ND	18	24	4	25	2	10	66	12	ND
R3	ND	19	25	6	27	2	7	66	14	ND
Day 5										
R1	ND	ND	ND	5	ND	1	ND	ND	93	ND
R2	ND	ND	ND	3	ND	2	ND	ND	95	ND
R3	ND	ND	ND	6	ND	3	ND	ND	88	3
Day 32										
R1	ND	ND	ND	ND	ND	1	ND	ND	99	ND
R2	ND	ND	ND	ND	ND	3	ND	ND	97	ND
R3	ND	ND	ND	ND	ND	1	ND	ND	99	ND

Results indicated that hydrolysis was one of the main degradation pathways. This is evidenced by the formation of 3-hydroxypropanal. 3-hydroxypropanal was then further oxidised to produce 3-hydropropionic acid. The biotransformation of acrolein under aerobic conditions was also demonstrated, as evidenced by the formulation of acrylic acid and allyl alcohol. This microbial biotransformation of acrolein took place early in the study and competed with the hydrolysis process. Acrolein also underwent rapid self-oxidation and reduction to produce its

Section 7.1.2.2.1 Annex Point IIIA XII 2.1	Aerobic aquatic degradation	
	oxidative product, acrylic acid and its reductive product, allyl alcohol. Acrylic acid was reduced to propionic and which oxidised to oxalic acid and eventually to carbon dioxide through complete mineralization. The fate of allyl alcohol was less obvious largely due to its volatility. For the same reason, allyl alcohol was not present in the aqueous phase in the same amount as acrylic acid. All metabolites of acrolein are polar and highly water soluble and are less volatile than acrolein. Due to the rapid degradation of acrolein through these pathways, the loss of radioactivity through volatility of acrolein was further inhibited. After 32 days, most of the remaining radioactivity was detected in the aqueous phase of the test system at approximately 25 % of the initial dose, while the radioactivity in the sediment phase amounted to approximately 20% of the initial dose. The decrease in radioactivity in the aqueous phase was not a result of sorption to solids but rather due to the rapid mineralization of acrolein metabolites to carbon dioxide Consequently, the carbon dioxide formed was found to be the major product in volatile traps. The mineralization of acrolein also took place in the sediment phase. Inorganic bicarbonate and carbonate anions absorbed strongly to the sediment which explains why the more non-polar solvents (e.g., acetonitrile, methanol) were not suitable for extracting sediment samples.	X
5.3 Conclusion	Results of this study indicated hydrolysis was an early step in acrolein degradation, and is supported by previous reported acrolein behaviour. Under the conditions of this study, acrolein underwent rapid hydrolysis and biodegradation in water.	
5.3.1 Reliability	1	
5.3.2 Deficiencies	No	

	Evaluation by Competent Authorities	
	Use separate "evaluation boxes" to provide transparency as to the comments and views submitted	
	EVALUATION BY RAPPORTEUR MEMBER STATE	
Date	30/11/2007	

Materials and Methods

The Applicant's version is acceptable, noting the following;

3.1.1 The sample number given in the summary (6587) differs from that stated in the study (6687).

3.1.3 The purity stated in the summary, 95.06%, is that reported by Sigma Aldrich. The Applicant's laboratory, SLI, states the purity to be 92.2%. The UK CA considers 92.2% the actual purity to be used.

3.3.3 There is no inclusion, in the summary, of the water and sediment characteristics. These are available in the study, however. The UK CA suggests the following tables to be included:

Table 1: Kern County Canal Sediment Characteristics:

Classification	Sand (%)	Silt (%)	Clay (%)	Field Moisture Capacity @ 0.33 bar (%)	PH	Cation Exchange (meq/100 g)	Organic Matter (%)	Bulk Density (disturbed) (gm/cc)
Sandy Loam	75	19	6	16.8	6.1	18.0	0.5	1.11

Table 2 : Kern County Canal Water Characteristics:

Description	Total Alkalinity (mg/L as $CaCO_3$)	Total Hardness (mg/L as $CaCO_3$)	Suspended Solids (mg/L)	Total Solids (mg/L)	Dissolved Oxygen (mg/L)	Ph (20°C)	Specific Conductivity (µ MHO/cm)
Clear/Yellow Tint	75	56	<0.002	0.122	10.8	8.0	184

3.3.6 EPA Guideline 162-04 states that the duration of the test is to be 30 days.

3.3.10 No controls were used.

<table>
<tr><td>Results and discussion</td><td>The Applicant's version is considered to be acceptable, noting the following;

5.2 No half-life data have been reported in the summary. These are available in the study, however. The UK CA suggests the following table to be included:

Table 3: Acrolein rate constants and half-life results for aerobic water samples:
<table><tr><th>No. Of Observations</th><th>Correlation Coefficient (r^2)</th><th>Rat Constant (1/hour)</th><th>Half-Life (hours)</th></tr><tr><td>12</td><td>0.994</td><td>0.021</td><td>33.7</td></tr></table>
Also, in the text it states '3-hydroxypropanal was then further oxidised to produce 3-hydropropionic acid'. The UK CA suggests this is changed to '3-hydroxypropanal was then further oxidised to produce 3-hydro<u>xy</u>propionic acid'.

Further in the text it is stated 'Acrylic acid was reduced to propionic and which oxidised to oxalic acid and eventually to carbon dioxide through complete mineralization.' The UK CA suggests this should read as follows:

'Acrylic acid was reduced to propionic <u>acid</u> and which oxidised to oxalic acid and eventually to carbon dioxide through complete mineralization.'

5.2 The last paragraph states 'After 32 days, most of the remaining radioactivity was detected in the aqueous phase of the test system at approximately 25 % of the initial dose, while the radioactivity in the sediment phase amounted to approximately 20% of the initial dose. The decrease in radioactivity in the aqueous phase was not a result of sorption to solids but rather due to the rapid mineralization of acrolein metabolites to carbon dioxide', this is a direct contradiction of the conclusions made by the Applicant regarding adsorption/desorption (section A7.1.3).</td></tr>
<tr><td>Conclusion</td><td>The Applicant's version is considered acceptable.</td></tr>
<tr><td>Reliability</td><td>2</td></tr>
<tr><td>Acceptability</td><td>Acceptable

No controls were used in the study, therefore the reliability factor has been changed to 2.</td></tr>
<tr><td>Remarks</td><td>All endpoints and data presented in the summary have been checked against the original study and are correct.</td></tr>
<tr><td></td><td>COMMENTS FROM ... (specify)</td></tr>
<tr><td>Date</td><td>Give date of comments submitted</td></tr>
<tr><td>Materials and Methods</td><td>Discuss additional relevant discrepancies referring to the (sub)heading numbers and to applicant's summary and conclusion.
Discuss if deviating from view of rapporteur member state</td></tr>
<tr><td>Results and discussion</td><td>Discuss if deviating from view of rapporteur member state</td></tr>
<tr><td>Conclusion</td><td>Discuss if deviating from view of rapporteur member state</td></tr>
<tr><td>Reliability</td><td>Discuss if deviating from view of rapporteur member state</td></tr>
<tr><td>Acceptability</td><td>Discuss if deviating from view of rapporteur member state</td></tr>
<tr><td>Remarks</td><td></td></tr>
</table>

Table A7_1_2_1_2-1: Inoculum / Test organism

Criteria	Details
Nature	Not specified
Species	Not specified
Strain	Not specified
Source	Canal
Sampling site	Kern County Canal, California, USA.
Laboratory culture	No
Method of cultivation	Not applicable
Preparation of inoculum for exposure	Upon receipt, the sediment was stored in the dark in a soil incubator maintained at 17 °C and subsequently sieved through a 2 mm stainless steel sieve. The canal water was refrigerated upon receipt.
Pretreatment	A daily 30 minute air purge of test systems allowed ample oxygenation yet deterred material loss.
Initial cell concentration	Water: 9.7×10^4 (CFU/ml) Sediment: 3.1×10^6 (CFU/ml)

Table A7_1_2_1_2-2: Test system

Criteria	Details
Culturing apparatus	Glass 1000 ml Erlenmeyer flask fitted with a glass Dreschel cap containing inlet and outlet ports for air exchange.
Number of replicates/concentration	3
Measuring equipment	For each test vessel, one Tenax® trap was used to collect the volatile products in series with two sodium hydroxide traps designed to collect ^{14}C-carbon dioxide.
Oxidation reduction indicator	No

Table A7_1_2_1_2-3: Test conditions

Criteria	Details
Composition of medium	Not specified
Additional substrate	No
Solvent	No
Preparation of medium	Each test vessel was covered with aluminium foil and incubated in an environmental chamber.
Test temperature	25 ± 1 °C
pH	Sediment: 6.1 Water: 8.0
Suspended solids concentration	< 0.002 mg/l
Other relevant criteria	Each sample was swirled after dosing

Section 7.1.2.2.2 Annex Point IIIA XII 2.1		Water/sediment degradation	
		1 REFERENCE	**Official use only**
1.1	**Reference**	Smith, A.M. (1993b), (^{14}C-Acrolein) - Determination of the Anaerobic Aquatic Metabolism, Springborn Laboratories, Inc. SLI Report No. 91-3-3680.	
1.2	**Data protection**	Yes	
1.2.1	Data owner	Baker Petrolite	
1.2.2	Criteria for data protection	Data on new a.s. for first entry to Annex I	
		2 GUIDELINES AND QUALITY ASSURANCE	
2.1	**Guideline study**	Yes US EPA FIFRA Guideline No. 162-3, 40 CFR 158.290	
2.2	**GLP**	Yes	
2.3	**Deviations**	Yes The protocol stated that a Beckman Model LS-1801 liquid scintillation counter would be used for LSC analyses. In this study, a Beckman Model LS-5000 liquid scintillation counter was also used in addition to the Beckman Model LS-1801 liquid scintillation counter. This deviation is not expected to alter the results of this study.	
		3 METHOD	
3.1	**Test material**	As given in Section 2	
3.1.1	Lot/Batch number	Sample No. 5587	X
3.1.2	Specification	As given in Section 2	
3.1.3	Purity	95.06 %	X
3.1.4	Further relevant properties	Acrolein has a water solubility of 23.7% at 25°C.	
3.1.5	Composition of Product	Not applicable	
3.1.6	TS inhibitory to micro-organisms	Yes Exposure to increasing concentrations of acrolein had increasingly inhibitory effects upon the population of *Anabaena flos-aquae*. The effects of test substance on mean standing crop on Day 5, relative to control, ranged from 5.12% to 98.6% inhibition.	
3.1.7	Specific chemical analysis	None used	
3.2	**Reference substance**	No	
3.2.1	Initial concentration of reference substance		
3.3	**Testing procedure**		

Section 7.1.2.2.2 Annex Point IIIA XII 2.1		Water/sediment degradation	
3.3.1	Inoculum / test species	*See Table A7_1_2_1_2-1*	
3.3.2	Test system	*See Table A7_1_2_1_2-2*	
3.3.3	Test conditions	*See Table A7_1_2_1_2-3*	X
3.3.4	Method of preparation of test solution	A radiolabelled super-stock solution was prepared by quantitatively transferring the entire contents of an ampoule of radiolabelled ^{14}C-acrolein (100 mCi) through repetitive rinsing with Burdick and Jackson high purity acetone into a 100 ml volumetric flask and diluting to volume. This super-stock had a mean measured concentration of 4.30 mg/ml by triplicate liquid scintillation counting (LSC) analyses. 2.50 ml of the 4.30 mg/ml radiolabelled stock was combined with 64.3 mg of non-radiolabelled acrolein and diluted to a final volume of 50 ml with NANOpure® water, to obtain a dosing solution concentration of 1.50 mg/ml acrolein. 4.00 ml of this solution was added by gas-tight syringe to each 1 litre flask replicate test vessel containing sediment and 400 ml of canal water to obtain a nominal concentration of 15.0 mg/l. 1.00 ml of this solution was added to each 250 ml flask replicate test vessel containing sediment and 100 ml of canal water to obtain a nominal test concentration of 15.0 mg/l.	
3.3.5	Initial TS concentration	15.0 mg/l	
3.3.6	Duration of test	184 days	
3.3.7	Analytical parameter	Rate of metabolism and pattern of decline of ^{14}C-acrolein.	
3.3.8	Sampling	Four 1 litre flasks, Replicates 11 – 14, were prepared and aqueous samples (10 ml) were drawn and analysed at Days 0, 1, 2 and 8. On Day 30 each complete 1 litre test system was collected and analysed. Ten 250 ml flasks, Replicates 1 - 10, were also prepared on Day 0 and two complete test systems were collected and both analysed at Days 93 and at Day 178. The sodium hydroxide trapping systems were replaced and analysed at Days 1, 2, 3, 4, 5, 7, 8, 11, 16, 21 and 28 for each 1 litre and 250 ml test system. Additional trap changes for the 250 ml test systems occurred on Days 36, 42, 49, 56, 63, 70, 85, 106, 119, 126, 142, 154, 168 and 178. Duplicate 250 ml test systems were collected at Days 93 and 178. (Replicates 2, 3 and 4, 5, respectively). At Day 30, the entire sample (both water and sediment) was centrifuged at 100 rpm for 20 minutes. The water fraction was sampled high performance liquid chromatography (HPLC) and radiometric LSC analysis. The sediment was removed for radiometric combustion analysis, microbial biomass determination and percent moisture analysis. Sub-samples of the sediment were extracted using sodium hydroxide and analysed by HPLC-RAM and LSC techniques. On Days 93 and 178, the canal water was decanted from samples of the test system and radiometric combustion analysis and percent moisture analysis was performed on the remaining sediment. Extracts were also analysed by HPLC-RAM and LSC techniques. The sodium hydroxide trapping systems were analysed by LSC over the course of the study to preclude saturation. Representative traps were chosen (Replicate 2 from Days 1 through 93 and Replicate 4 from days 106 through 178) and analysed by barium hydroxide precipitation procedure to determine the presence of ^{14}C -carbon dioxide. In addition, Day 30 (Replicate 13) canal water and Day 93 (Replicate 2) and Day 178	

Section 7.1.2.2.2 Annex Point IIIA XII 2.1	Water/sediment degradation	
	(Replicate 4) canal water and sediment were also analysed. The resulting precipitate was filtered and analysed by LSC along with the supernatant. The Day 178 (Replicate 4) post extraction sediment was acidified to test for bicarbonate content.	
3.3.9 Intermediates/ degradation products	Identified High performance liquid chromatography with radiometric detection (HPLC-RAM) revealed the following degradation products: Day 1- oxalic acid Day 2- acrylic acid, allyl alcohol and 3-hydroxypropionic acid Day 8- 3-hydroxypropanal, propanol and propionic acid All of these metabolites were further mineralised to carbon dioxide	
3.3.10 Controls	Not specified	X
3.3.11 Statistics	A cumulative material balance was calculated for each 1litre replicate at each sampling interval and a final material balance was calculated on Day 30 for the 1 litre replicates and Days 93 and 178 for the 250 ml replicates. The material balance was calculated by summing the cumulative disintegrations per minute (DPM) recovered in the carbon dioxide and Tenax® traps, DPM recovered in the canal water, DPM recovered in the sediment extract, and the non-extractable DPM remaining in the sediment, and then dividing by the total DPM applied in the dose.	
	4 RESULTS	
4.1 Degradation of test substance		
4.1.1 Degradation of TS in abiotic control	Not specified	
4.1.2 Degradation	Carbon dioxide, the primary degradation product, was formed in the water phase on Day 2 and remained throughout the study. Expressed as bicarbonate ion (HCO_3^-), carbon dioxide represented greater than 60% of HPLC-RAM peak area on Days 30, 93 and 178. On the Day 8, 30, 93 and 178 sampling events, carbon dioxide was observed to be 13% (1.5 ppm acrolein equivalents), 20% (2.4 ppm acrolein equivalents) 4.4% (0.5 ppm acrolein equivalents) and 3.2% (0.4 ppm acrolein equivalents) of the initial dose, respectively.	

Section 7.1.2.2.2 Annex Point IIIA XII 2.1	Water/sediment degradation	
4.1.3 Graph		
	Figure 1: Cumulative Data from Traps	
4.1.4 Other observations	None	
4.1.5 Degradation of reference substance	Not applicable	
4.1.6 Intermediates/ degradation products	See Section 5.2 Through Day 2 of the study, three products were produced in the water phase which were ephemeral in nature: acrylic acid, allyl alcohol and 3-hydropropionic acid. Through Day 8 of the study, three products were produced in the water phase which were detected at trace levels by Day 30 of the study: 3-hydroxypropanal, propanol and propionic acid. Additionally, oxalic acid was formed on Day 1 and remained throughout the study. All of these metabolites were further mineralised to carbon dioxide	
	5 APPLICANT'S SUMMARY AND CONCLUSION	
5.1 Materials and methods	US EPA FIFRA Guideline No. 162-3 The protocol stated that a Beckman Model LS-1801 liquid scintillation counter would be used for LSC analyses. In this study, a Beckman Model LS-5000 liquid scintillation counter was also used in addition to the Beckman Model LS-1801 liquid scintillation counter. This deviation is not expected to alter the results of this study.	
5.2 Results and discussion	HPLC results of canal water samples as percent of peak area	X

HPLC results of canal water samples as percent of peak area

	Acrolein	3-hydroxy propanal	acrylic acid	allyl alcohol	propionic acid	oxalic acid	3-hydroxy propionic acid	sum	bi-carb-onate	propanal
Day 0										
R11	62	7	17	15	ND	ND	ND	ND	ND	ND
R12	29	5	48	17	ND	1	ND	ND	ND	ND
R13	62	9	14	15	ND	0 5	ND	ND	ND	ND
R14	66	9	13	12	ND	ND	ND	ND	ND	ND
Day 1										
R11	ND	6	46	13	24	1	6	67	ND	7
R12	ND	4	57	13	19	2	4	74	ND	4
R13	ND	6	36	23	29	1	2	56	ND	13
R14	ND	10	30	25	25	2	4	42	ND	17

Section 7.1.2.2.2 Water/sediment degradation
Annex Point IIIA XII 2.1

Day 2										
R11	ND	3	33	6	43	2	ND	87	12	3
R12	ND	2	53	6	33	2	ND	86	3	3
R13	ND	3	32	12	44	2	ND	70	4	8
R14	ND	2	23	14	50	2	ND	66	3	11
Day 8										
R11	ND	8	ND	ND	37	1	ND	87	55	2
R12	ND	4	ND	ND	91	1	ND	92	5	2
R13	ND	8	ND	ND	82	2	ND	89	11	1
R14	ND	7	ND	ND	72	3	ND	88	22	2
Day 30										
R11	ND	ND	ND	ND	ND	5	ND	ND	95	ND
R12	ND	1	ND	ND	70	1	ND	93	29	2
R13	ND	2	ND	ND	12	4	ND	89	82	5
R14	ND	ND	ND	ND	ND	6	ND	ND	94	ND
Day 93										
R2	ND	ND	ND	ND	ND	24	4	ND	61	ND
R3	ND	ND	ND	ND	ND	22	ND	ND	64	ND
Day 178										
R4	ND	ND	ND	ND	ND	30	ND	ND	70	ND
R5	ND	ND	ND	ND	ND	27	ND	ND	73	ND

Results indicated that hydrolysis was one of the main degradation pathways. This is evidenced by the formation of 3-hydroxypropanal. 3-hydroxypropanal was then further oxidised to produce 3-hydropropionic acid. The biotransformation of acrolein under anaerobic conditions was also demonstrated, as evidenced by the formulation of allyl alcohol. This microbial biotransformation of acrolein took place early in the study and competed with the hydrolysis process. Acrolein also underwent rapid self-oxidation and reduction to produce its oxidative product, acrylic acid and its reductive product, allyl alcohol during the early stages of the study. Allyl alcohol was then further reduced to propanol and acrylic acid was further reduced to propionic acid. All of these transient metabolites were then further metabolised under anaerobic conditions to their and products, carbon dioxide and oxalic acid.

All metabolites of acrolein are polar and highly water soluble and are less volatile than acrolein. After 30 days, most of the remaining radioactivity was detected in the aqueous phase of the test system at approximately 29% of the initial dose, while the radioactivity in the sediment phase amounted to approximately 22% of the initial dose. By Day 93, most of the remaining radioactivity was detected in the sediment phases of the test system at 20% of initial dose, while the radioactivity in the aqueous phase amounted to approximately 7.0% of the initial dose. On Day 178, the radioactivity remaining in the aqueous phase was 5% of the initial dose and in the sediment was 11% of the initial dose. The observed decrease in radioactivity in the aqueous phase was a result of sorption to solids and also due to the rapid mineralization of acrolein metabolites to carbon dioxide. Consequently, the carbon dioxide formed was found to be the major product in volatile traps. The mineralization of acrolein also took place in the sediment phase. Inorganic bicarbonate and carbonate anions absorbed strongly to the sediment which explains why the more non-polar solvents (e.g., acetonitrile, methanol) were not suitable for extracting sediment samples.

5.3 Conclusion

Results of this study indicated hydrolysis was an early step in acrolein degradation, and is supported by previous reported acrolein behaviour. Under the conditions of this study, acrolein underwent rapid hydrolysis and biodegradation in water.

5.3.1 Reliability: 1 — X

Section 7.1.2.2.2 Annex Point IIIA XII 2.1	Water/sediment degradation	
5.3.2 Deficiencies	Yes See Section 2.3	
	Evaluation by Competent Authorities	
	Use separate "evaluation boxes" to provide transparency as to the comments and views submitted	

EVALUATION BY RAPPORTEUR MEMBER STATE

Date

09/05/2006

Materials and Methods

The Applicant's version is considered acceptable, noting the following;

3.1.1 The sample number in the summary (5587) is different from the one stated in the study (6687). The UKCA suggests that the following should be included:

- Non-radiolabelled Acrolein, Lot No. 6687
- Radiolabelled Acrolein, Lot no. 032H9223

3.1.3 The purity stated in the summary (95.06) is that of the study sponsored non-radiolabelled Acrolein. The radiolabelled Acrolein purity should also be included. The UKCA suggests point 3.1.3 should read:

- Non-radiolabelled Acrolein (reported by study sponsor) = 95.06%
- Radiolabelled Acrolein = ~95% (Sigma Chemicals Company), and 92.2% (duplicate radiochemical purity performed at SLI)

3.3.3 There is no inclusion, in the summary, of the water and sediment characteristics. These are available in the study, however. The UK CA suggests the following tables to be included:

Table 1: Kern County Canal Sediment Characteristics:

Classification	Sand (%)	Silt (%)	Clay (%)	Field Moisture Capacity @ 0.33 bar (%)	PH	Cation Exchange (meq/100 g)	Organic Matter (%)	Bulk Density (disturbed) (gm/cc)
Sandy Loam	75	19	6	16.8	6.1	18.0	0.5	1.11

Table 2: Kern County Canal Water Characteristics:

Description	Total Alkalinity (mg/L as $CaCO_3$)	Total Hardness (mg/L as $CaCO_3$)	Suspended Solids (mg/L)	Total Solids (mg/L)	Dissolved Oxygen (mg/L)	Ph (20°C)	Specific Conductivity (µ MHO/cm)
Clear/Yellow Tint	75	56	<0.002	0.122	10.8	8.0	184

3.3.10 No controls were used.

Section 7.1.2.2.2 **Annex Point IIIA XII 2.1**	**Water/sediment degradation**
Results and discussion	The Applicant's Version is considered acceptable, noting the following; **5.2** The data presented within the report demonstrates that Acrolein rapidly degraded with a half-life < 1 day (the interim report states 10.3 hours) under anaerobic aquatic conditions. The interim study also concluded that the half-life in sediment, based on radioactivity, was 240 hours (10 days)
Conclusion	The Applicant's version is considered to be acceptable
Reliability	2
Acceptability	Acceptable No controls were specified; therefore the reliability factor has been changed to 2.
Remarks	All endpoints and data presented in the summary have been checked against the original study and are correct.
	COMMENTS FROM ... *(specify)*
Date	*Give date of comments submitted*
Materials and Methods	*Discuss additional relevant discrepancies referring to the (sub)heading numbers and to applicant's summary and conclusion.* *Discuss if deviating from view of rapporteur member state*
Results and discussion	*Discuss if deviating from view of rapporteur member state*
Conclusion	*Discuss if deviating from view of rapporteur member state*
Reliability	*Discuss if deviating from view of rapporteur member state*
Acceptability	*Discuss if deviating from view of rapporteur member state*
Remarks	

Table A7_1_2_1_2-1: Inoculum / Test organism

Criteria	**Details**
Nature	Not specified
Species	Not specified
Strain	Not specified
Source	Canal
Sampling site	Kern Island Canal, California, USA.
Laboratory culture	No
Method of cultivation	Not applicable
Preparation of inoculum for exposure	Upon receipt, the sediment was stored in the dark in a soil incubator maintained at 17 °C and subsequently sieved through a 2 mm stainless steel sieve. The canal water was refrigerated upon receipt.
Pretreatment	Test vessels containing untreated sediment and water were anaerobically incubated for approximately one month prior to dosing by daily 30 minute purging with

	nitrogen.
Initial cell concentration	Water: 2.2 x 10^2 (CFU/ml) Sediment: 8.3 x 10^5 (CFU/ml)

Table A7_1_2_1_2-2: Test system

Criteria	Details
Culturing apparatus	Glass Erlenmeyer flask (1000 or 250 ml) fitted with a glass Dreschel cap containing inlet and outlet ports for nitrogen exchange.
Number of replicates/concentration	14
Measuring equipment	For each test vessel, one Tenax® trap was used to collect the volatile products in series with two sodium hydroxide traps designed to collect ^{14}C-carbon dioxide
Oxidation reduction indicator	No

Table A7_1_2_1_2-3: Test conditions

Criteria	Details
Composition of medium	To promote microbial oxygen consumption and maintain an anaerobic environment, test vessels were flooded with 400 ml (1 litre test systems) or 100 ml (250 ml test systems) of a 1% glucose/canal water solution.
Additional substrate	No
Solvent	No
Preparation of medium	Each test vessel was covered with aluminium foil and incubated in an environmental chamber kept at 25 ± 1 °C.
Test temperature	Not specified
pH	7.96
Suspended solids concentration	< 0.002 mg/l
Other relevant criteria	Each sample was swirled after dosing

Section A7.1.3 Annex Point IIA7.7		Adsorption test	
		1 REFERENCE	Official use only
1.1	**Reference**	Irwin, K (1988) Soil Adsorption Coefficient for Acrolein (Magnacide®Herbicide and Magnacide®B Microbiocide). SRI International. SRI Project No. 3562-2.	
1.2	**Data protection**	Yes	
1.2.1	Data owner	Baker Petrolite	
1.2.2	Criteria for data protection	Data on new a.s for first entry to Annex I	
		2 GUIDELINES AND QUALITY ASSURANCE	
2.1	**Guideline study**	Yes FIFRA No. 163-1	
2.2	**GLP**	Yes	
2.3	**Deviations**	No	
		3 MATERIALS AND METHODS	
3.1	**Test material**	As given in Section 2	X
3.1.1	Lot/Batch number	NN-481-76	
3.1.2	Specification	As given in Section 2	X
3.1.3	Purity	See 3.1.2.	
3.1.4	Further relevant properties	The test material will hydrolyse in water as well as polymerise in the presence of light. The test was conducted in 24 hours to minimise these effects	X
3.1.5	Method of analysis	Acrolein concentration was determined by either ultraviolet absorption spectroscopy or HPLC analysis. The absorbance was measured in a 1cm cuvette with a Beckman DU-2 spectrophotometer at 209 nm. A stock solution of Acrolein was prepared by pippetting 100 µl of Acrolein into 500 ml of argon-sparged deionised water. Serial dilutions of the stock solutions were prepared to generate the calibration curve from absorbance versus concentration. Dilutions of sorption samples and the calibration solutions were prepared in 10 ml flask to give a final concentration less than 5 mg per litre Acrolein. Additional samples were prepared in the same manner using 0.01M calcium sulphate solution. The calibration curve was determined from single determinations at five concentrations for both the deionised water and calcium sulphate solutions. HPLC conditions: Instrument: Waters model 6000A liquid chromatograph Mobile phase: 30% acetonitrile/70% water Flow rate: 1 ml/min Injection size: 5 µl Column: C18 Since Acrolein undergoes hydration in water, the Acrolein solutions used in the sorption experiments were analysed before and after the sorption equilibration period. Duplicate injections of the solutions gave reproducible results (<1%), therefore it was necessary to analyse the	X

Section A7.1.3 Annex Point IIA7.7		Adsorption test	
		sample as soon as possible.	
3.2	**Degradation products**	No.	X
3.2.1	Method of analysis for degradation products		
3.3	**Reference substance**	None.	
3.3.1	Method of analysis for reference substance		
3.4	**Soil types**	see table A7_1 _3-1	X
3.5	**Testing procedure**		
3.5.1	Test system	To prevent volatilisation of Acrolein, experiments were conducted with Turlock soil using continuous-flow frontal analysis. The soil column (4 mm i.d. stainless steel, 8 cm long) was packed with 1.6g of autoclaved Turlock soil between silanised glass wool and 5µ stainless steel frits. The column was conditioned with deionised water to remove water-soluble leachates.	X
3.5.2	Test solution and Test conditions		X
3.6	**Test performance**		
3.6.1	Preliminary test	No.	
3.6.2	Screening test: Adsorption	No.	
3.6.3	Screening test: Desorption		X
3.6.4	HPLC-method	A Waters LC system which includes a WISP 710B autosampler, the Programmable System Controller and Data Module, and Model 450 Variable Wavelength Detector was used. The flow rate was 1mL/min and injection size was 5µL.	
3.6.5	Other test		
		4 RESULTS	
4.1	**Preliminary test**		
4.2	**Screening test: Adsorption**		X
4.3	**Screening test: Desorption**		X
4.4	**Calculations**		
4.4.1	Ka , Kd	.Ka 0.14 to 1.26 mL/g	
4.4.2	Ka_{oc} , Kd_{oc}	Ka_{oc} 50 to 270 mL/g	
4.5	**Degradation product(s)**		X

Section A7.1.3 Annex Point IIA7.7		Adsorption test	
		5 APPLICANT'S SUMMARY AND CONCLUSION	
5.1	**Materials and methods**	The study was conducted according to FIFRA Guideline No. 163-1. The soil or sediment samples were weighed into 25 ml corex centrifuge tubes with Teflon-lined caps. The tubes were then filled to a zero headspace with six dilutions of the aqueous Acrolein solution. Appropriate soil and solution blanks at each concentration were run simultaneously with the sorption samples. The samples were equilibrated with end-over-end- mixing in a 25°C temperature-controlled air bath for four hours. Following equilibration, the samples were centrifuged at 25°C and 10,000 rpm for 20 minutes. The initial and final Acrolein concentrations in the solution phase were determined using either absorbance measurements at 209 nm, or HPLC analysis. The concentration of Acrolein on the soil or sediment was calculated from the difference between the equilibrium concentration of tubes with sorbent and the appropriate solution blank. A continuous-flow frontal analysis was used, the Acrolein solution or deionised water were percolated through the column at a constant flow rate (5.0 ml/min) with two HPLC syringe pumps connected to the column by four-way valve. The effluent flowed directly into a variable wavelength detector at 209 nm. A computer program was used to integrate the areas above the breakthrough and elution curves and to calculate the amounts adsorped and desorbed.	X
5.2	**Results and discussion**	Acrolein adsorption on autoclaved Turlock soil was too small to measure using batch adsorption measurements. In two sets of experiments the average changes in the aqueous concentration without soil were 22% and 14.5%, whereas in sample with soil the average changes were 21% and 13.5% respectively.	X
5.2.1	Adsorbed a.s. [%]		X
5.2.2	K_a	Ranging between 0.14 and 1.26 mL/g	X
5.2.3	K_d		
5.2.4	Ka_{oc}	Ranging between 50 and 270 mL/g	X
5.2.5	Ka/Kd		
5.2.6	Degradation products (% of a.s.)		X
5.3	**Conclusion**	The higher K_{oc} values and the irreversible sorption of Acrolein suggest that Acrolein specifically interacts with substrate mineral and organic carbon functional groups. The measured Kp values are insufficient to estimate Acrolein mobility through soils. Sorption irreversibility, hydration, biotransformation and volatilization are expected to significantly retard the high infiltration rates of Acrolein estimated from these low Kp values	X
5.3.1	Reliability	2	
5.3.2	Deficiencies	Yes. There are no desorbent values.	

Section A7.1.3 Annex Point IIA7.7	Adsorption test	
	Evaluation by Competent Authorities	
	Use separate "evaluation boxes" to provide transparency as to the comments and views submitted	
	EVALUATION BY RAPPORTEUR MEMBER STATE	
Date	21/04/2006	
Materials and Methods	The study report provided was poorly summarised but all relevant raw data and results were presented. The Applicant's evaluation of the available data was not adequate. However, the UKCA has reproduced essential results below where relevant to demonstrate that the study provided should be considered adequate for risk assessment purposes. The Applicant's version is unclear, the following additional points should be noted; **3.1 & 3.1.2** The purity (96.17 %) and specification reported in the study is very similar but not identical to that given in A2 (refers to Appendix XI Confidential data). However, the UK CA is confident that the study is valid for this endpoint. **3.1.4** There is no reference in the study for the statement 'It is also known that Acrolein will polymerize in the presence of light'. There is no evidence to support this statement in any of the photolytic degradation studies (DOC IIIA, 7.1.3 and 7.1.1.1.2), therefore it should be removed **3.2** Identification of degradation products was not performed. **3.4** Table A7_1_3-1 refers to 4 soils being used in the study; 1, 2, 3 and 4, which are referred to in the study as EPA-6 sediment, Turlock soil, Phoenix soil and Menlo Park soil respectively, **3.5.1** and **5.1** The summary information provided is unclear. This study was carried out in 2 parts. Firstly, partition coefficients were investigated for 3 soils and 1 sediment using 25 ml centrifuge tubes (as detailed under 5.1). Then in order to investigate the impact of volatilisation on the results from the primary test, the adsorption of acrolein was investigated further using continuous-flow frontal analysis for soil 2 (Turlock soil). See point 3.5.1 in summary for further details. The Applicant's summary and the study report state that the study was conducted to FIFRA Guideline No. 163-1. However, neither the study nor the summary states that the soil was aged under aerobic conditions prior to the test beginning. This is a requirement stated in EPA guideline 163-1.The soil column dimensions do not match those recommended by EPA guideline 163-1. The guideline states 'the column should be from 30 to 300 cm in height' not 8 cm as used for the continuous-flow frontal analysis.**3.6.3** No details were given in the report but results of batch desorption analysis were discussed (see **4.3** below).	

Section A7.1.3 Annex Point IIA7.7	Adsorption test
	3.5.2 Details of test conditions are provided below; a) Batch adsorption analysis The experiment was carried out using end-over mixing at 25°C for 4 hours.

Sample	Number of replicates		Mean sorbent conc. (±SD) (g/ml)	Acrolein conc. (initial min – max range)
	Soil	No soil		
Soil 1 (EPA-6 sediment)	10	12	0.18 (±0.003)	48 - 241
Soil 2 (Turlock soil)	9	7	0.33 (±0.01)	64 - 250
Soil 3 (Phoenix soil)	6	6	0.38 (±0.02)	2.8 - 97
Soil 4 (Menlo Park soil)	11	11	0.22 (±0.13)	4.22 – 96.5

b) Continuous flow sorption experiment with soil 2 (Turlock soil)

Experimental Conditions	
Temperature	25°C
Mass of soil	1.6257 g
Column dimensions	4 mm (internal diam.), 8 cm long
Solute	0.002 M $CaSO_4$
Flow rate	0.5 mL/min
Detector	Waters model 450 at 209 nm

Results and discussion

The Applicant's version is unacceptable and should be replaced by the following UK CA evaluation of available data;

4.3 The study report states that in batch desorption studies no acrolein was desorbed from the soil. **4.2, 5.2, 5.2.1, 5.2.2 & 5.2.4** The mean percentage adsorption/loss estimated from the difference between initial and final acrolein concentrations both with and without (blanks) the influence of soil have been calculated by the UK CA and are presented in the following Table;

Section A7.1.3 Annex Point IIA7.7	Adsorption test

Sample	% Adsorption/loss (±SD)		Overall mean % adsorption [adjusted for blank effects]
	Soil	No soil (blank)	
Soil 1 (EPA-6 sediment)	22.6 (±4.5)	13.6 (±3.9)	9.0
Soil 2 (Turlock soil)	17.2 (±5.3)	17.7 (±4.8)	-0.5*
Soil 3 (Phoenix soil)	26.2 (±3.8)	2.84 (±2.0)	23.35
Soil 4 (Menlo Park soil)	29.0 (±13.3)	9.9 (±11.0)	19.0

* - Turlock soil, greater losses were recorded for the blank solutions than those with soil.

Acrolein adsorption on autoclaved Turlock soil was too small to measure using batch adsorption measurements and the mean changes in the aqueous acrolein concentration without soil (blanks) were not significantly different from those with soil. For the remaining 3 soils there were small but significant differences between the with and without soil (blank) samples and adsorption coefficients were calculated. The following table presents the available regression parameters for the batch adsorption isotherms:

Sample	K_p (slope)	±SD	Corr. Coeff.	% OC	K_{oc}
Soil 1 (EPA-6 sediment)	0.93	0.05	0.99	0.72	130
Soil 3 (Phoenix soil)	0.73	0.03	0.99	0.27	270
Soil 4 (Menlo Park soil)	1.26	0.1	0.94	2.67	51

For the additional experiments using soil 2 (Turlock soil) with a continuous frontal flow sorption technique, the K_p and K_{oc} for acrolein were estimated to be 0.14 (± 0.03) mL/g and 52 mL/g.

4.5 and **5.2.6** From the available HPLC analysis data it would suggest that where degradation products were detected (additional peaks to acrolein) the levels were too small for quantification. Therefore, these metabolites would be less than 10 % of the applied parent compound and not of concern for the risk assessment.

Conclusion

The Applicant’s version is not acceptable for the following reasons;

5.3 There was no evidence presented to support that the Acrolein interacted with substrate mineral and carbonyl functional groups under the conditions tested. The study and Applicant’s summary was centred on the fact that the experimental Kp values being higher than those predicted, and no desorption could be detected. However, the data presented for the range of soils tested do not suggest adsorption is a main route of removal for acrolein. In addition, the available analytical data does not suggest that there are significant quantities of soluble metabolites formed. Therefore, volatilisation of acrolein or its metabolites from the system cannot be dismissed as supported by the improved adsorption data using the continuous flow technique for soil 2.

Section A7.1.3 Annex Point IIA7.7	Adsorption test	
	The UK CA has concluded from the data presented in the study report that acrolein has a strong tendency to remain in the aquatic phase, removal from which is likely to be predominantly via volatilisation or biodegradation.	
Reliability	2	
Acceptability	Acceptable	
Remarks	All endpoints addressed in the summary have been checked against those in the study. Although the information was poorly presented both in the original study and the Applicant's summary (e.g. tables A7_1 _3-2, A7_1 _3-3 and A7_1 _3-4 included, but not completed), the available raw data in the study has enabled the UK CA to evaluate this endpoint thoroughly. The UK CA has concluded that the overall endpoint is sufficiently robust for the risk assessment of acrolein considering its use is limited as a slimicide for offshore oil drilling. However, should acrolein be proposed for use where direct application/release to soil is expected, additional data to address soil mobility would be required.	
	COMMENTS FROM ...	
Date	*Give date of comments submitted*	
Materials and Methods	*Discuss additional relevant discrepancies referring to the (sub)heading numbers and to applicant's summary and conclusion.* *Discuss if deviating from view of rapporteur member state*	
Results and discussion	*Discuss if deviating from view of rapporteur member state*	
Conclusion	*Discuss if deviating from view of rapporteur member state*	
Reliability	*Discuss if deviating from view of rapporteur member state*	
Acceptability	*Discuss if deviating from view of rapporteur member state*	
Remarks		

Table A7_1 _3-1: Classification and physico-chemical properties of soils used as adsorbents

	Soil 1	Soil 2	Soil 3	Soil 4
Soil order				
Soil series				
Classification				
Location				
Horizon				
Sand [%]	0.2	87.7	61.4	46
Silt [%]	31.2	7.8	24.6	31.8
Clay [%]	68.6	4.5	14	22.2
Organic carbon [%]	0.72	0.27	0.27	2.7
Carbonate as calcium carbonate				
Insoluble carbonates [%]				
pH (1:1 water)	7.83	7.3	7.9	5.9
Cation exchange capacity (MEQ/100 g)	33.1	2.8	9.1	21.5
Extractable cations (MEQ/100 g)				
Calcium				
Magnesium				
Sodium				
Potassium				
Hydrogen				
Special chemical/mineralogical features				
Clay fraction mineralogy				

Table A7_1 _3-2: Results of preliminary test:

Test substance	
Sample purity	
Weighed soil	
Volume of calcium chloride solution	
Nominal concentration of a.s. final solution	
Analytical concentration final of a.s. solution	
Concentration of the test solution (show calculation)	
Details of the analytical method used:	
Method	
Recovery rate	
Detection limit	

Table A7_1 _3-3: Results of screening test - adsorption:

	Soil 1		Soil 2		Soil 3	
Concentration of test material [mg/l]						
After contact of....hours with soil						
Correction for blank with soil						
Correction for blank without soil						
Final corrected concentration [mg/l]						
Initial concentration of test solution [mg/l]						
Decrease in concentration [mg/l]						
Quantity adsorbed [µg]						
Quantity of soil [g of oven-dried equivalent]						
Quantity adsorbed [µg] per gram of soil						
Test material adsorbed [%]						
Temperature [°C]						
Volume of solution recovered after centrifugation [ml]						
Volume of solution not recovered [ml]						
Corresponding quantity of test substance [mg]						

Table A7_1 _3-4: Results of screening test - desorption:

	Soil 1		Soil 2		Soil 3	
Temperature [°C]						
Concentration in combined washings [mg/l]						
Corresponding quantity of test material [mg]						
Quantity desorbed [µg]						
[%] of adsorbed test material, which is desorbed						
[%] of adsorbed test material, which is not desorbed						

Section A7.1.3 **Annex Point IIA VII.7.7**	**Adsorption/desorption screening test**	
	JUSTIFICATION FOR NON-SUBMISSION OF DATA	**Official use only**
Other existing data [X] **Limited exposure [ ]**	**Technically not feasible [ ]** **Scientifically unjustified [ ]** **Other justification [ ]**	
Detailed justification:	A screening study is not required as a determination of absorption in soil has been performed. See section IIIA7.3.1.	
Undertaking of intended data submission [ ]		
	Evaluation by Competent Authorities	
	Use separate "evaluation boxes" to provide transparency as to the comments and views submitted	
	EVALUATION BY RAPPORTEUR MEMBER STATE	
Date	18/05/2006	
Evaluation of applicant's justification	The Applicant's justification is acceptable	
Conclusion	Acceptable	
Remarks		
	COMMENTS FROM OTHER MEMBER STATE *(specify)*	
Date	*Give date of comments submitted*	
Evaluation of applicant's justification	*Discuss if deviating from view of rapporteur member state*	
Conclusion	*Discuss if deviating from view of rapporteur member state*	
Remarks		

Section A7.1.3 Annex Point IIA7.7	Adsorption test	
	1 REFERENCE	Official use only
1.1 Reference	Irwin, K (1988) Soil Adsorption Coefficient for Acrolein (Magnacide®Herbicide and Magnacide®B Microbiocide). SRI International. SRI Project No. 3562-2.	
1.2 Data protection	Yes	
1.2.1 Data owner	Baker Petrolite	
1.2.2 Criteria for data protection	Data on new a.s for first entry to Annex I	
	2 GUIDELINES AND QUALITY ASSURANCE	
2.1 Guideline study	Yes FIFRA No. 163-1	
2.2 GLP	Yes	
2.3 Deviations	No	
	3 MATERIALS AND METHODS	
3.1 Test material	As given in Section 2	X
3.1.1 Lot/Batch number	NN-481-76	
3.1.2 Specification	As given in Section 2	X
3.1.3 Purity	See 3.1.2.	
3.1.4 Further relevant properties	The test material will hydrolyse in water as well as polymerise in the presence of light. The test was conducted in 24 hours to minimise these effects	X
3.1.5 Method of analysis	Acrolein concentration was determined by either ultraviolet absorption spectroscopy or HPLC analysis. The absorbance was measured in a 1cm cuvette with a Beckman DU-2 spectrophotometer at 209 nm. A stock solution of Acrolein was prepared by pippetting 100 µl of Acrolein into 500 ml of argon-sparged deionised water. Serial dilutions of the stock solutions were prepared to generate the calibration curve from absorbance versus concentration. Dilutions of sorption samples and the calibration solutions were prepared in 10 ml flask to give a final concentration less than 5 mg per litre Acrolein. Additional samples were prepared in the same manner using 0.01M calcium sulphate solution. The calibration curve was determined from single determinations at five concentrations for both the deionised water and calcium sulphate solutions. HPLC conditions: Instrument: Waters model 6000A liquid chromatograph Mobile phase: 30% acetonitrile/70% water Flow rate: 1 ml/min Injection size: 5 µl Column: C18 Since Acrolein undergoes hydration in water, the Acrolein solutions used in the sorption experiments were analysed before and after the sorption equilibration period. Duplicate injections of the solutions gave reproducible results (<1%), therefore it was necessary to analyse the	X

Section A7.1.3 Annex Point IIA7.7		Adsorption test	
		sample as soon as possible.	
3.2	**Degradation products**	No.	X
3.2.1	Method of analysis for degradation products		
3.3	**Reference substance**	None.	
3.3.1	Method of analysis for reference substance		
3.4	**Soil types**	see table A7_1 _3-1	X
3.5	**Testing procedure**		
3.5.1	Test system	To prevent volatilisation of Acrolein, experiments were conducted with Turlock soil using continuous-flow frontal analysis. The soil column (4 mm i.d. stainless steel, 8 cm long) was packed with 1.6g of autoclaved Turlock soil between silanised glass wool and 5µ stainless steel frits. The column was conditioned with deionised water to remove water-soluble leachates.	X
3.5.2	Test solution and Test conditions		X
3.6	**Test performance**		
3.6.1	Preliminary test	No.	
3.6.2	Screening test: Adsorption	No.	
3.6.3	Screening test: Desorption		X
3.6.4	HPLC-method	A Waters LC system which includes a WISP 710B autosampler, the Programmable System Controller and Data Module, and Model 450 Variable Wavelength Detector was used. The flow rate was 1mL/min and injection size was 5µL.	
3.6.5	Other test		
		4 RESULTS	
4.1	**Preliminary test**		
4.2	**Screening test: Adsorption**		X
4.3	**Screening test: Desorption**		X
4.4	**Calculations**		
4.4.1	Ka , Kd	.Ka 0.14 to 1.26 mL/g	
4.4.2	Ka_{oc} , Kd_{oc}	Ka_{oc} 50 to 270 mL/g	
4.5	**Degradation product(s)**		X

Section A7.1.3 Annex Point IIA7.7	Adsorption test	
	5 APPLICANT'S SUMMARY AND CONCLUSION	
5.1 Materials and methods	The study was conducted according to FIFRA Guideline No. 163-1. The soil or sediment samples were weighed into 25 ml corex centrifuge tubes with Teflon-lined caps. The tubes were then filled to a zero headspace with six dilutions of the aqueous Acrolein solution. Appropriate soil and solution blanks at each concentration were run simultaneously with the sorption samples. The samples were equilibrated with end-over-end- mixing in a 25°C temperature-controlled air bath for four hours. Following equilibration, the samples were centrifuged at 25°C and 10,000 rpm for 20 minutes. The initial and final Acrolein concentrations in the solution phase were determined using either absorbance measurements at 209 nm, or HPLC analysis. The concentration of Acrolein on the soil or sediment was calculated from the difference between the equilibrium concentration of tubes with sorbent and the appropriate solution blank. A continuous-flow frontal analysis was used, the Acrolein solution or deionised water were percolated through the column at a constant flow rate (5.0 ml/min) with two HPLC syringe pumps connected to the column by four-way valve. The effluent flowed directly into a variable wavelength detector at 209 nm. A computer program was used to integrate the areas above the breakthrough and elution curves and to calculate the amounts adsorped and desorbed.	X
5.2 Results and discussion	Acrolein adsorption on autoclaved Turlock soil was too small to measure using batch adsorption measurements. In two sets of experiments the average changes in the aqueous concentration without soil were 22% and 14.5%, whereas in sample with soil the average changes were 21% and 13.5% respectively.	X
5.2.1 Adsorbed a.s. [%]		X
5.2.2 K_a	Ranging between 0.14 and 1.26 mL/g	X
5.2.3 K_d		
5.2.4 Ka_{oc}	Ranging between 50 and 270 mL/g	X
5.2.5 Ka/Kd		
5.2.6 Degradation products (% of a.s.)		X
5.3 Conclusion	The higher K_{oc} values and the irreversible sorption of Acrolein suggest that Acrolein specifically interacts with substrate mineral and organic carbon functional groups. The measured Kp values are insufficient to estimate Acrolein mobility through soils. Sorption irreversibility, hydration, biotransformation and volatilization are expected to significantly retard the high infiltration rates of Acrolein estimated from these low Kp values	X
5.3.1 Reliability	2	
5.3.2 Deficiencies	Yes. There are no desorbent values.	

Section A7.1.3 Annex Point IIA7.7	Adsorption test	
	Evaluation by Competent Authorities	
	Use separate "evaluation boxes" to provide transparency as to the comments and views submitted	
	EVALUATION BY RAPPORTEUR MEMBER STATE	
Date	21/04/2006	
Materials and Methods	The study report provided was poorly summarised but all relevant raw data and results were presented. The Applicant's evaluation of the available data was not adequate. However, the UKCA has reproduced essential results below where relevant to demonstrate that the study provided should be considered adequate for risk assessment purposes. The Applicant's version is unclear, the following additional points should be noted; **3.1 & 3.1.2** The purity (96.17 %) and specification reported in the study is very similar but not identical to that given in A2 (refers to Appendix XI Confidential data). However, the UK CA is confident that the study is valid for this endpoint. **3.1.4** There is no reference in the study for the statement 'It is also known that Acrolein will polymerize in the presence of light'. There is no evidence to support this statement in any of the photolytic degradation studies (DOC IIIA, 7.1.3 and 7.1.1.1.2), therefore it should be removed **3.2** Identification of degradation products was not performed. **3.4** Table A7_1_3-1 refers to 4 soils being used in the study; 1, 2, 3 and 4, which are referred to in the study as EPA-6 sediment, Turlock soil, Phoenix soil and Menlo Park soil respectively, **3.5.1** and **5.1** The summary information provided is unclear. This study was carried out in 2 parts. Firstly, partition coefficients were investigated for 3 soils and 1 sediment using 25 ml centrifuge tubes (as detailed under 5.1). Then in order to investigate the impact of volatilisation on the results from the primary test, the adsorption of acrolein was investigated further using continuous-flow frontal analysis for soil 2 (Turlock soil). See point 3.5.1 in summary for further details. The Applicant's summary and the study report state that the study was conducted to FIFRA Guideline No. 163-1. However, neither the study nor the summary states that the soil was aged under aerobic conditions prior to the test beginning. This is a requirement stated in EPA guideline 163-1.The soil column dimensions do not match those recommended by EPA guideline 163-1. The guideline states 'the column should be from 30 to 300 cm in height' not 8 cm as used for the continuous-flow frontal analysis.**3.6.3** No details were given in the report but results of batch desorption analysis were discussed (see **4.3** below).	

Section A7.1.3 Annex Point IIA7.7	Adsorption test

3.5.2 Details of test conditions are provided below;

a) Batch adsorption analysis

The experiment was carried out using end-over mixing at 25°C for 4 hours.

Sample	Number of replicates		Mean sorbent conc. (±SD) (g/ml)	Acrolein conc. (initial min – max range)
	Soil	No soil		
Soil 1 (EPA-6 sediment)	10	12	0.18 (±0.003)	48 - 241
Soil 2 (Turlock soil)	9	7	0.33 (±0.01)	64 - 250
Soil 3 (Phoenix soil)	6	6	0.38 (±0.02)	2.8 - 97
Soil 4 (Menlo Park soil)	11	11	0.22 (±0.13)	4.22 – 96.5

b) Continuous flow sorption experiment with soil 2 (Turlock soil)

Experimental Conditions	
Temperature	25°C
Mass of soil	1.6257 g
Column dimensions	4 mm (internal diam.), 8 cm long
Solute	0.002 M $CaSO_4$
Flow rate	0.5 mL/min
Detector	Waters model 450 at 209 nm

Results and discussion

The Applicant's version is unacceptable and should be replaced by the following UK CA evaluation of available data;

4.3 The study report states that in batch desorption studies no acrolein was desorbed from the soil. **4.2, 5.2, 5.2.1, 5.2.2 & 5.2.4** The mean percentage adsorption/loss estimated from the difference between initial and final acrolein concentrations both with and without (blanks) the influence of soil have been calculated by the UK CA and are presented in the following Table;

Section A7.1.3 Annex Point IIA7.7	Adsorption test

Sample	% Adsorption/loss (±SD)		Overall mean % adsorption [adjusted for blank effects]
	Soil	No soil (blank)	
Soil 1 (EPA-6 sediment)	22.6 (±4.5)	13.6 (±3.9)	9.0
Soil 2 (Turlock soil)	17.2 (±5.3)	17.7 (±4.8)	-0.5*
Soil 3 (Phoenix soil)	26.2 (±3.8)	2.84 (±2.0)	23.35
Soil 4 (Menlo Park soil)	29.0 (±13.3)	9.9 (±11.0)	19.0

* - Turlock soil, greater losses were recorded for the blank solutions than those with soil.

Acrolein adsorption on autoclaved Turlock soil was too small to measure using batch adsorption measurements and the mean changes in the aqueous acrolein concentration without soil (blanks) were not significantly different from those with soil. For the remaining 3 soils there were small but significant differences between the with and without soil (blank) samples and adsorption coefficients were calculated. The following table presents the available regression parameters for the batch adsorption isotherms:

Sample	K_p (slope)	±SD	Corr. Coeff.	% OC	K_{oc}
Soil 1 (EPA-6 sediment)	0.93	0.05	0.99	0.72	130
Soil 3 (Phoenix soil)	0.73	0.03	0.99	0.27	270
Soil 4 (Menlo Park soil)	1.26	0.1	0.94	2.67	51

For the additional experiments using soil 2 (Turlock soil) with a continuous frontal flow sorption technique, the K_p and K_{oc} for acrolein were estimated to be 0.14 (± 0.03) mL/g and 52 mL/g.

4.5 and **5.2.6** From the available HPLC analysis data it would suggest that where degradation products were detected (additional peaks to acrolein) the levels were too small for quantification. Therefore, these metabolites would be less than 10 % of the applied parent compound and not of concern for the risk assessment.

Conclusion

The Applicant's version is not acceptable for the following reasons;

5.3 There was no evidence presented to support that the Acrolein interacted with substrate mineral and carbonyl functional groups under the conditions tested. The study and Applicant's summary was centred on the fact that the experimental Kp values being higher than those predicted, and no desorption could be detected. However, the data presented for the range of soils tested do not suggest adsorption is a main route of removal for acrolein. In addition, the available analytical data does not suggest that there are significant quantities of soluble metabolites formed. Therefore, volatilisation of acrolein or its metabolites from the system cannot be dismissed as supported by the improved adsorption data using the continuous flow technique for soil 2.

Section A7.1.3 **Annex Point IIA7.7**	**Adsorption test**	
Reliability	The UK CA has concluded from the data presented in the study report that acrolein has a strong tendency to remain in the aquatic phase, removal from which is likely to be predominantly via volatilisation or biodegradation. 2	
Acceptability	Acceptable	
Remarks	All endpoints addressed in the summary have been checked against those in the study. Although the information was poorly presented both in the original study and the Applicant's summary, the available raw data in the study has enabled the UK CA to evaluate this endpoint thoroughly. The UK CA has concluded that the overall endpoint is sufficiently robust for the risk assessment of acrolein considering its use is limited as a slimicide for offshore oil drilling. However, should acrolein be proposed for use where direct application/release to soil is expected, additional data to address soil mobility would be required.	
	COMMENTS FROM ...	
Date	*Give date of comments submitted*	
Materials and Methods	*Discuss additional relevant discrepancies referring to the (sub)heading numbers and to applicant's summary and conclusion.* *Discuss if deviating from view of rapporteur member state*	
Results and discussion	*Discuss if deviating from view of rapporteur member state*	
Conclusion	*Discuss if deviating from view of rapporteur member state*	
Reliability	*Discuss if deviating from view of rapporteur member state*	
Acceptability	*Discuss if deviating from view of rapporteur member state*	
Remarks		

Table A7_1 _3-1: Classification and physico-chemical properties of soils used as adsorbents

	Soil 1	Soil 2	Soil 3	Soil 4
Soil order				
Soil series				
Classification				
Location				
Horizon				
Sand [%]	0.2	87.7	61.4	46
Silt [%]	31.2	7.8	24.6	31.8
Clay [%]	68.6	4.5	14	22.2
Organic carbon [%]	0.72	0.27	0.27	2.7
Carbonate as calcium carbonate				
Insoluble carbonates [%]				
pH (1:1 water)	7.83	7.3	7.9	5.9
Cation exchange capacity (MEQ/100 g)	33.1	2.8	9.1	21.5
Extractable cations (MEQ/100 g)				
Calcium				
Magnesium				
Sodium				
Potassium				
Hydrogen				
Special chemical/mineralogical features				
Clay fraction mineralogy				

Table A7_1 _3-2: Results of preliminary test:

Test substance	
Sample purity	
Weighed soil	
Volume of calcium chloride solution	
Nominal concentration of a.s. final solution	
Analytical concentration final of a.s. solution	
Concentration of the test solution (show calculation)	
Details of the analytical method used:	
Method	
Recovery rate	
Detection limit	

Table A7_1 _3-3: Results of screening test - adsorption:

	Soil 1		Soil 2		Soil 3	
Concentration of test material [mg/l]						
After contact of....hours with soil						
Correction for blank with soil						
Correction for blank without soil						
Final corrected concentration [mg/l]						
Initial concentration of test solution [mg/l]						
Decrease in concentration [mg/l]						
Quantity adsorbed [µg]						
Quantity of soil [g of oven-dried equivalent]						
Quantity adsorbed [µg] per gram of soil						
Test material adsorbed [%]						
Temperature [°C]						
Volume of solution recovered after centrifugation [ml]						
Volume of solution not recovered [ml]						
Corresponding quantity of test substance [mg]						

Table A7_1 _3-4: Results of screening test - desorption:

	Soil 1		**Soil 2**		**Soil 3**	
Temperature [°C]						
Concentration in combined washings [mg/l]						
Corresponding quantity of test material [mg]						
Quantity desorbed [µg]						
[%] of adsorbed test material, which is desorbed						
[%] of adsorbed test material, which is not desorbed						

Section A7.1.4 **Annex Point IIIA XII.2.2**	**Further studies on adsorption and desorption in water/sediment systems and, where relevant, on the adsorption and desorption of metabolites and degradation products where the preliminary risk assessment indicates that it is necessary**	
	JUSTIFICATION FOR NON-SUBMISSION OF DATA	**Official use only**
Other existing data [ ] **Limited exposure [ ]**	**Technically not feasible [ ]** **Scientifically unjustified [X]** **Other justification [ ]**	
Detailed justification:	Radiolabelled studies on the degradation of the active substance and its metabolites in water and sediment have been performed with absorption/desorption studies in sediment (Section IIIA7.1.2.1.1, IIIA7.1.2.1.2). Further studies on adsorption and desorption in water/sediment systems and on the adsorption and desorption of metabolites and degradation products, are not considered to be necessary.	
Undertaking of intended data submission [ ]		
	Evaluation by Competent Authorities	
	Use separate "evaluation boxes" to provide transparency as to the comments and views submitted	
	EVALUATION BY RAPPORTEUR MEMBER STATE	
Date	18/05/2006	
Evaluation of applicant's justification	The Applicant's justification is acceptable	
Conclusion	Acceptable	
Remarks		
	COMMENTS FROM OTHER MEMBER STATE *(specify)*	
Date	*Give date of comments submitted*	
Evaluation of applicant's justification	*Discuss if deviating from view of rapporteur member state*	
Conclusion	*Discuss if deviating from view of rapporteur member state*	
Remarks		

Section A7.1.4.1 Annex Point IIIA XII.2.1	Field study on accumulation in the sediment	
	JUSTIFICATION FOR NON-SUBMISSION OF DATA	**Official use only**
Other existing data [ ] **Limited exposure [ ]**	**Technically not feasible [ ]** **Scientifically unjustified [X]** **Other justification [ ]**	
Detailed justification:	Further studies on accumulation in the sediment are not considered necessary as the active substance has been shown to be easily dissimilated in a ready biodegradation study (Section A7.1.1.2.1, Annex Point IIA, VII.7.6.1.1.). In addition the active substance has been shown to undergo rapid degradation by physico-chemical processes including rapid volatilisation (A7.2.1) and photodegradation (A7.1.1.1.2) and microbial degradation in water (anaerobic and aerobic freshwater-sediment radio-labelled studies, A7.1.2.1.1 and A7.1.2.1.2) transforming the active substance to CO2.	
Undertaking of intended data submission [ ]		
	Evaluation by Competent Authorities	
	Use separate "evaluation boxes" to provide transparency as to the comments and views submitted	
	EVALUATION BY RAPPORTEUR MEMBER STATE	
Date	18/05/2006	
Evaluation of applicant's justification	The Applicant's justification is acceptable	
Conclusion	Acceptable	
Remarks		
	COMMENTS FROM OTHER MEMBER STATE *(specify)*	
Date	*Give date of comments submitted*	
Evaluation of applicant's justification	*Discuss if deviating from view of rapporteur member state*	
Conclusion	*Discuss if deviating from view of rapporteur member state*	
Remarks		

Section A7.2.1 Annex Point IIA7.4, 7.1.1		Fate and behaviour in soil: aerobic degradation in soil	
		1 REFERENCE	**Official use only**
1.1	**Reference**	Chou, T-W. & Spanggord, R.J. (1990) Estimation of the Aerobic Biotransformation Rates for Acrolein (Magnacide®H Herbicide, Magnacide®B Microbiocide) in Soil. SRI International. SRI Project No. 2562-4.	
1.2	**Data protection**	Yes	
1.2.1	Data owner	Baker Petrolite	
1.2.2	Criteria for data protection	Data on new a.s. for first entry to Annex I	
		2 GUIDELINES AND QUALITY ASSURANCE	
2.1	**Guideline study**	Yes FIFRA 162-1	
2.2	**GLP**	No No GLP statement	X
2.3	**Deviations**	No	
		3 MATERIALS AND METHODS	
3.1	**Test material**	As given in Section 2	
3.1.1	Lot/Batch number	NN-481-76	
3.1.2	Specification	As given in Section 2 Deviating from specification given in section 2 as follows Radiolabelled at the 2 and 3 positions (acrolein-2,3-^{14}C)	
3.1.3	Purity	See 3.1.2	
3.1.4	Further relevant properties		
3.1.5	Method of analysis		
3.2	**Degradation products**	Degradation products tested: Yes/No	X
3.2.1	Method of analysis for degradation products	At various time points, three tubes (one sterile and two non-sterile) were used, 9.0 ml of acetonitrile (Burdick & Jackson, HPLC grade) added, and the suspension was vigorously shaken by hand for five minutes. The tubes were centrifuged at 2500 rpm for 10 minutes and the acetonitrile (plus 1.2 ml water originally added) was pipetted into a vial and capped. The soil was transferred to a sintered glass funnel, washed with acetone, filtered, and air-dried. The acetonitrile extracts were analysed by high-performance liquid chromatography (HPLC) using the following conditions: Instrument: Spectra-Physics Model 8000 Liquid Chromatograph Column: Regis Hi-Chrom ODS-II column, 4.7 x 250 mm	

Section A7.2.1 Annex Point IIA7.4, 7.1.1	Fate and behaviour in soil: aerobic degradation in soil	
	Solvent: Water/Acetonitrile (80/20) Flow rate: 1.0 ml/minute Detectors: UV at 210 nm in series with a Raytest solid-state radioactivity detector Quantitation was achieved using the external standard method relation peak area to parts per million (ppm) of acrolein injected as determined from standard calibration curves. Total radioactivity in the extract was determined by direct counting of a 50 µl aliquot diluted in Aquasol scintillation counting liquid. The soil samples were oxidised using a Packard Model 306 Oxidizer where the sample is combusted and the ^{14}C-carbon is converted to ^{14}C-carbon dioxide and trapped. The trapped activity is counted in a scintillation counter.	
3.3 Reference substance	No	
3.3.1 Method of analysis for reference substance	Not applicable	
3.4 Soil types	See table A7_2_1-1	
3.5 Testing procedure		
3.5.1 Test system	Studies were performed in 20 x 150 mm Pyrex glass tubes capped with Teflon liners. 36 tubes were prepared by weighing 10.0 g of Phoenix soil into each tube. 0.8ml of deionised water (67% of field capacity) was added to each tube, and the contents were thoroughly mixed with a metal spatula. The tubes were allowed to stand at room temperature (20 - 22°C) for seven days to activate microbial populations. 12 tubes were autoclaved for one hour on each of three consecutive days to serve as sterile controls. 0.5 ml of sterile water was added to each sterile tube after autoclaving to re supply the water lost on heating.	
3.5.2 Test solution and Test conditions	**Biotransformation rate studies:** A stock solution of ^{14}C-acrolein in water was prepared by adding 0.37 ml of the solution (3.3 mCi in 0.5 ml of dimethylformamide, further diluted to 1.0 ml with acetonitrile) to 29.6 ml of sterilised water (total volume = 30 ml). 0.4 ml of this solution was added to the sterile and non-sterile tubes containing 10g of soil, to yield a 10 ppm acrolein spike with respect to the soil [(56 mg/8.9 mCi) x (3.3 mCi x 0.37 ml/30 ml) x 0.4 ml] = 0.10 mg/10 g soil]. This aqueous addition brought the total soil moisture content up to 75% of field capacity. The soil was mixed with a spatula and capped to minimise volatisation. One sterile and two non-sterile tubes were removed for extraction and analysis at times 0, 2, 4, 8, 48 and 115 hours after application. The study was conducted at 20 - 23°C. **Mineralisation studies:** Conducted in three 250 ml Bartha biometer flasks. 50 g of soil was added to each flask (three Phoenix soil flasks) and 4.0 ml of deionised water. The soils were thoroughly mixed and allowed to acclimate for seven	

Section A7.2.1 Annex Point IIA7.4, 7.1.1		Fate and behaviour in soil: aerobic degradation in soil	
		days. One flask was autoclaved for one hour each on three consecutive days to serve as a sterile control. To each flask side arm was added 10 ml 0.2M potassium hydroxide solution to trap evolved carbon dioxide. 2.0 ml of the aqueous acrolein stock solution was added to each flask and the contents thoroughly mixed. The potassium hydroxide solution was replaced with fresh solution at Days 2, 6, 13, 20, 27, and 34. A 50 µl aliquot of the potassium hydroxide solution was mixed with 10 ml of Aquasol counting solution for scintillation counting. A 5.0 ml aliquot was mixed with 5.0 ml of 0.2M barium chloride solution to precipitate carbon dioxide. After centrifuging the precipitate, a 100 µl aliquot was mixed with the counting solution for scintillation counting. The difference between the potassium hydroxide and barium chloride solution counts was attributed to ^{14}C-carbon dioxide.	
3.6	**Test performance**		
3.6.1	Identification of products	Products were identified by their co-chromatography with authentic standards or as derivatised products. Two derivatisation procedures were used; One procedure involved the conversion of aldehydes to their pentafluorophenylhydrazones by reaction with pentafluorophenylhydrazine. The derivatives were then analysed be HPLC as described in section 3.2.1 with the exception that gradient program was used starting from acetonitrile/water (20/80) for 5 minutes programmed to 100% acetonitrile in five minutes (six minute hold). The column was re-equilibrated for five minutes with the starting solvent composition. The components, 3-hydroxypropanal pentafluorophenylhydrazone and acrolein pentafluorophenylhydrazone eluted at 12.5 and 14.5 minutes respectively. To confirm, identifications were performed by gas chromatography/mass spectroscopy using a Ribermag R-10-10 GC/MS and a 30 m DB-5 fused silica capillary temperature programmed from 50 - 200°C	
3.6.2	Analysis of Data	The loss of acrolein from soil was assumed to a following a first-order reaction shown in Equation 1: **Equation 1** $-d[A]/dt = k_b [A]$ Where: [A] = Concentration of acrolein k_b = First-order biotransformation rate constant t = time. Integration of Equation 1 yields Equation 2 **Equation 2** $\ln [A_o]/[A_t] = k_b t$ Where: $[A_o]$ = Concentration of acrolein at time zero $[A_t]$ = Concentration at time t. Other loss processes (irreversible sorption, hydrolysis and volatilization) are occurring to acrolein on soil besides biotransformation. The half life	

Section A7.2.1 Annex Point IIA7.4, 7.1.1	Fate and behaviour in soil: aerobic degradation in soil	
	of acrolein in soil due to biotransformation : $t½ = \ln 2/k_b$	
3.6.3 Screening test: Desorption	Not performed	
3.6.4 HPLC-method	According to (a)" OECD-HPLC-method": Yes/No	X
	4 RESULTS	
4.1 Preliminary test	The extraction of acrolein from low moisture field capacity (unsaturated) soils was poor, with only 75 - 77% recovered after the initial mixing. This is due to both water and acrolein competing for available binding sites on the soil. As the water is adsorbed, acrolein is volatilised due to its increased concentration in the aqueous phase, the high soil surface area to liquid ratio, and the mixing of the tube contents.	
4.2 Biotransformation Rate	Acrolein was found to be rapidly lost from both the sterile and non-sterile Phoenix soil reaction tubes. Acrolein was completely gone from the acetonitrile extracts within 8 hours in the non-sterile soils and within 115 hours in the sterile soils. The non-sterile soils followed first-order kinetics. The average rate constant was $0.431 \pm 0.08\ hr^{-1}$. The sterile soil did not show first-order behaviour, it mimicked that observed for reversible first-order processes up to 48 hours. The average first-order rate constant for the sterile soils was $0.264\ hr^{-1}$. The rate constant for the aerobic soil biotransformation was $0.167\ hr^{-1}$, thus the aerobic soil biotransformation half-life was 4.2 hours. The uncorrected half-life of acrolein in soil is approximately 1.4 hours. Acrolein Loss in Aerobic Soil PPM Acrolein Time (hrs) PPM-S PPM-NS1 PPM-NS2 NS = nonsterile Figure 1. Acrolein (ppm) loss as a function of time in Sterile and Non-sterile soils	
4.3 Products	Two products were identified; 1. Acrylic acid: – CH_2=CH-COOH, formed in sterile soil, but there was approximately twice the amount in the non-sterile soil. The disappearance rate is similar for both types of soil. This was totally removed after 115 hours in sterile soil. 2. 3-hydroxypropionic acid: – HO-CH_2-CH_2-COOH, disappears rapidly in the non-sterile soils to where it is non-detectable after	

<table>
<tr><td>Section A7.2.1
Annex Point IIA7.4, 7.1.1</td><td colspan="3">Fate and behaviour in soil: aerobic degradation in soil</td><td></td></tr>
<tr><td></td><td colspan="3">48 hours.
3. Carbon dioxide: – formed rapidly within the seven days and shows a more gradual release up till the termination of the study.
In the sterile control soil, 3-hydroxypropanal was present as a result from the hydrolysis of acrolein. This was not present in the non-sterile soil.</td><td></td></tr>
<tr><td rowspan="6">4.4 Material balance</td><td colspan="3">The total material balance was 98.3%. The data below show the distribution of activity found in material balance</td><td rowspan="6"></td></tr>
<tr><td>Sample</td><td>Activity found (x 10^{-6} dpm)</td><td>% of Total</td></tr>
<tr><td>Soil extract</td><td>12.5</td><td>43.1</td></tr>
<tr><td>Plug extract</td><td>2.87</td><td>9.9</td></tr>
<tr><td>Soil</td><td>5.66</td><td>19.5</td></tr>
<tr><td>Plug</td><td>7.98</td><td>27.5</td></tr>
<tr><td>4.5 Binding to soil</td><td colspan="3">The recovery of acrolein from soil was low indicating that other loss processes were occurring simultaneously with biotransformation. One such process was irreversible binding to the soil. At least 27.5% of the activity readily binds to the soil and is not extracted by acetonitrile, water, or 0.2M sodium hydroxide solution after a 20 minute exposure to the soil. In non-sterile soils, the binding of acrolein and products is complete after 8 hours followed by an observed loss of activity with time. The activity bound to the soil after 8 hours represents 109% (due to volatilised acrolein adding back to the soil) of the total activity added.
The sterile soil showed less total binding of activity than the non-sterile soils and the activity appeared to remain constant after 8 hours.</td><td></td></tr>
<tr><td>4.5.1 Conversion of soil bound products</td><td colspan="3">Carbon dioxide generated from acrolein, acrolein metabolites, and acrolein bound to soil was followed as a function of time by measuring the activity trapped in 0.2M potassium hydroxide solution and by precipitating the ^{14}C-carbon dioxide with barium chloride and recounting the solution.
The majority of the activity was released within several days and approximately 50% of the released activity was carbon dioxide. After six days, the released activity was entirely carbon dioxide and appeared to follow a zero-order release rate upto the end of the study.
Between zero and six days, acrolein and other volatile metabolites that are trapped in 0.2M potassium hydroxide are released from soil. This indicates that the irreversibly bound acrolein products are converted to carbon dioxide and this transformation is biotic.</td><td></td></tr>
<tr><td></td><td colspan="3">5 APPLICANT'S SUMMARY AND CONCLUSION</td><td></td></tr>
<tr><td>5.1 Materials and methods</td><td colspan="3">This study was conducted in accordance to FIFRA Guideline No. 162-1.
Soil biotransformation rate study were performed in 20 x 150 mm Pyrex glass tubes capped with Teflon liners. 36 tubes were prepared by weighing 10.0 g of Phoenix soil into each tube. 0.8 ml of deionised water (67% of field capacity) was added to each tube, and the contents were thoroughly mixed with a metal spatula. The tubes were allowed to stand</td><td></td></tr>
</table>

Section A7.2.1 Annex Point IIA7.4, 7.1.1	Fate and behaviour in soil: aerobic degradation in soil	
	at room temperature (20 - 22°C) for seven days to activate microbial populations. 12 tubes were autoclaved for one hour on each of three consecutive days to serve as sterile controls. 0.5 ml of sterile water was added to each sterile tube after autoclaving to re supply the water lost on heating.	
5.2 Results and discussion	Acrolein is shot-lived when added to unsaturated soils and its fate will be controlled by biotransformation, volatilisation and irreversible binding to soil processes. Free acrolein in soil is readily biotransformed with a half-life of 4.2 hours. Acrylic acid and 3-hydroxypropionic acid are also readily biotransformed and are presumably converted to carbon dioxide with a half-life of 29 days. Acrolein products that are irreversibly bound to soil are mineralised to carbon dioxide with an estimated half-life of 410 days. The bound products are not readily extracted from soil since they are not even solubilised by 0.2M sodium hydroxide. The transformations of acrolein in soil produce polar products that are rapidly consumed (within 48 hours) but at a slower rate than acrolein. The mechanism by which acrolein irreversibly binds to soil in inconclusive, since even the normal procedure for removing fulvic and humic acids from soil failed to significantly remove the majority of bound radioactivity. The bound materials are biodegradable and can be mineralised to carbon dioxide.	X
5.3 Conclusion	Biotransformation of acrolein and its abiotic transformation products will occur readily in aerobic soil eventually leading to carbon dioxide. Based on the rapid evolution of carbon dioxide, it appears that soil microbes adapt easily to concentrations above any expected field exposure value. Thus, microbes will play an important role in the overall persistence of acrolein in soil.	
5.3.1 Reliability	1	
5.3.2 Deficiencies	No	
	Evaluation by Competent Authorities	
	Use separate "evaluation boxes" to provide transparency as to the comments and views submitted	
	EVALUATION BY RAPPORTEUR MEMBER STATE	
Date	16/07/2007 The Applicant's version is considered acceptable, noting the following; **2.2** There is no certificate of GLP, which has been noted by the applicant.	
Materials and Methods	The Applicant's version is considered acceptable, noting the following; **3.2** Should read 'Degradation products tested: Yes' **3.6.4** Should read 'According to (a) "OECD-HPLC-method": Yes'	

Section A7.2.1 **Annex Point** IIA7**.4, 7.1.1**	**Fate and behaviour in soil: aerobic degradation in soil**
Results and discussion	The Applicant's version is considered acceptable, noting the following: **5.2** The first line states: 'Acrolein is **shot**-lived when added….', this is a spelling error and should be replaced with 'Acrolein is **short**-lived when added…'. The Applicant has not discussed the issue of volatilisation from the initial soil samples. Data presented in the study show that approximately 50 % of the applied radioactivity (AR) was recovered in the NaOH traps but that only 35 % of this was CO_2. Data available in the study also suggests that the bound fraction within the soil was approximately 30 % radioactive residues by the end of the study (115 h). Although the Applicant identified 2 main metabolites, these were not quantified. Acrylic acid exceeded 10 % of the AR after 4 hours with a mean peak of 14.7 % AR recorded at 48 hours in non-sterile soil. By 115 hours no acrylic acid was detected in either the sterile or non-sterile soils tested. The second degradation product discussed by the applicant, 3-hydroxypropionic acid did not exceed a mean of 10 % AR under non-sterile soil with a maximum peak value of 9.4 % AR reported after 2 hours, which declined to zero by 48 hours. This is therefore not a substance for concern in the risk assessment.
Conclusion	The Applicant's version is considered acceptable.
Reliability	2
Acceptability	Acceptable The reliability factor has been changed to 2 because there is no certificate of GLP (This has been noted by the Applicant). However, it should be noted that the study was started in 1989, which is the year in which GLP use began, hence GLP certification may not have been readily available at this time. The UKCA believes that the data reported in the study are sufficiently robust for risk assessment.
Remarks	All endpoints and data presented in the summary have been checked against the original study and are correct. The UK CA notes that the Applicant has included uncompleted tables within the study summary (A7_2 _1-3, A7_2 _1-4, A7_2 _1-2). This will not affect the reliability factor of the study.
	COMMENTS FROM ...
Date	*Give date of comments submitted*
Materials and Methods	*Discuss additional relevant discrepancies referring to the (sub)heading numbers and to applicant's summary and conclusion.* *Discuss if deviating from view of rapporteur member state*
Results and discussion	*Discuss if deviating from view of rapporteur member state*
Conclusion	*Discuss if deviating from view of rapporteur member state*
Reliability	*Discuss if deviating from view of rapporteur member state*
Acceptability	*Discuss if deviating from view of rapporteur member state*
Remarks	

Table A7_2 _1-1: Classification and physico-chemical properties of soils used as adsorbents

	Soil 1
Soil identification	Pheonix
Classification	Sandy loam
Location	Cotton field located at S.32nd Street in Phoenix, Arizona, USA
Sand [%]	61.4
Silt [%]	24.6
Clay [%]	14.0
Organic matter [%]	0.4
pH (1:1 H_2O)	7.9
Cation exchange capacity (MEQ/100 g)	9.1

Table A7_2 _1-2: Results of preliminary test:

Test substance	
Sample purity	
Weighed soil	
Volume of $CaCl_2$ solution	
Nominal concentration of a.s. final solution	
Analytical concentration final of a.s. solution	
Concentration of the test solution (show calculation)	
Details of the analytical method used:	
Method	
Recovery rate	
Detection limit	

Table A7_2 _1-3: Results of screening test - adsorption:

	Soil 1	
Concentration of test material [mg/l]		
After contact of....hours with soil		
Correction for blank with soil		
Correction for blank without soil		
Final corrected concentration [mg/l]		
Initial concentration of test solution [mg/l]		
Decrease in concentration [mg/l]		
Quantity adsorbed [µg]		
Quantity of soil [g of oven-dried equivalent]		
Quantity adsorbed [µg] per gram of soil		
Test material adsorbed [%]		
Temperature [°C]		
Volume of solution recovered after centrifugation [ml]		
Volume of solution not recovered [ml]		
Corresponding quantity of test substance [mg]		

Table A7_2 _1-4: Results of screening test - desorption:

	Soil 1	
Temperature [°C]		
Concentration in combined washings [mg/l]		
Corresponding quantity of test material [mg]		
Quantity desorbed [µg]		
[%] of adsorbed test material, which is desorbed		
[%] of adsorbed test material, which is not desorbed		

Section A7.2.2.1 Annex Point IIIA VII.4, XII.1.1, XII.1.4	The rate and route of degradation including identification of the process involved and identification of any metabolites and degradation products in at least three soil types under appropriate conditions	
	JUSTIFICATION FOR NON-SUBMISSION OF DATA	**Official use only**
Other existing data [ ] **Limited exposure [X]**	**Technically not feasible [ ]** **Scientifically unjustified [X]** **Other justification [ ]**	
Detailed justification:	The use pattern of acrolein would lead to negligible exposure to soil. The rate and route of degradation in soil has already been elucidated in studies on the estimation of the aerobic biotransformation rates for acrolein (Magnacide®H Herbicide, Magnacide®B Microbiocide) in soil (Section A7.2.1, Annex Point IIIA, VII.4., Ann. IIIA, XII.1.1.) and the soil adsorption coefficient for acrolein (Magnacide®Herbicide and Magnacide®B Microbiocide) study (Section A7.1.3, Annex Point IIIA, XII.2.2.) Therefore, in view of the low exposure potential in soil from use and the existing data further studies are considered not to be necessary.	
Undertaking of intended data submission [ ]		

	Evaluation by Competent Authorities
	Use separate "evaluation boxes" to provide transparency as to the comments and views submitted
	EVALUATION BY RAPPORTEUR MEMBER STATE
Date	18/05/2006
Evaluation of applicant's justification	The Applicant's justification is acceptable
Conclusion	Acceptable
Remarks	
	COMMENTS FROM OTHER MEMBER STATE *(specify)*
Date	*Give date of comments submitted*
Evaluation of applicant's justification	*Discuss if deviating from view of rapporteur member state*
Conclusion	*Discuss if deviating from view of rapporteur member state*
Remarks	

Section A7.2.2.2 **Annex Point IIIA XII.1.1, Annex VI, para 85**	**Field soil dissipation and accumulation**	
	JUSTIFICATION FOR NON-SUBMISSION OF DATA	**Official use only**
Other existing data [ ] **Limited exposure [X]**	**Technically not feasible [ ]** **Scientifically unjustified [X]** **Other justification [ ]**	
Detailed justification:	The use pattern of acrolein would lead to negligible exposure to soil. The rate and route of degradation in soil has already been elucidated in studies on the estimation of the aerobic biotransformation rates for acrolein (Magnacide®H Herbicide, Magnacide®B Microbiocide) in soil (Section A7.2.1, Annex Point IIIA, VII.4., Ann. IIIA, XII.1.1.) and the soil adsorption coefficient for acrolein (Magnacide®Herbicide and Magnacide®B Microbiocide) study (Section A7.1.3, Annex Point IIIA, XII.2.2.) Therefore, in view of the low exposure potential in soil from use and the existing data further studies are considered not to be necessary	
Undertaking of intended data submission [ ]		

	Evaluation by Competent Authorities
	Use separate "evaluation boxes" to provide transparency as to the comments and views submitted
	EVALUATION BY RAPPORTEUR MEMBER STATE
Date	18/05/2006
Evaluation of applicant's justification	The Applicant's justification is acceptable.
Conclusion	Acceptable
Remarks	
	COMMENTS FROM OTHER MEMBER STATE *(specify)*
Date	*Give date of comments submitted*
Evaluation of applicant's justification	*Discuss if deviating from view of rapporteur member state*
Conclusion	*Discuss if deviating from view of rapporteur member state*
Remarks	

Section A7.2.2.3 **Annex Point IIIA XII.1.4**	**Extent and nature of bound residues**	
	JUSTIFICATION FOR NON-SUBMISSION OF DATA	**Official use only**
Other existing data [ ] **Limited exposure [X]**	**Technically not feasible [ ]** **Scientifically unjustified [X]** **Other justification [ ]**	
Detailed justification:	The use pattern of acrolein would lead to negligible exposure to soil. The rate and route of degradation in soil has already been elucidated in studies on the estimation of the aerobic biotransformation rates for acrolein (Magnacide®H Herbicide, Magnacide®B Microbiocide) in soil (Section A7.2.1, Annex Point IIIA, VII.4., Ann. IIIA, XII.1.1.) and the soil adsorption coefficient for acrolein (Magnacide®Herbicide and Magnacide®B Microbiocide) study (Section A7.1.3, Annex Point IIIA, XII.2.2.) Therefore, in view of the low exposure potential in soil from use and the existing data further studies are considered not to be necessary	
Undertaking of intended data submission [ ]		
	Evaluation by Competent Authorities	
	Use separate "evaluation boxes" to provide transparency as to the comments and views submitted	
	EVALUATION BY RAPPORTEUR MEMBER STATE	
Date	18/05/2006	
Evaluation of applicant's justification	The Applicant's justification is acceptable.	
Conclusion	Acceptable	
Remarks		
	COMMENTS FROM OTHER MEMBER STATE *(specify)*	
Date	*Give date of comments submitted*	
Evaluation of applicant's justification	*Discuss if deviating from view of rapporteur member state*	
Conclusion	*Discuss if deviating from view of rapporteur member state*	
Remarks		

Section A7.2.2.3 **Annex Point IIIA XII.1.4**	**Extent and nature of bound residues**	
	JUSTIFICATION FOR NON-SUBMISSION OF DATA	**Official use only**

Section A7.2.2.3 **Annex Point IIIA XII.1.4**	**Extent and nature of bound residues**	
Other existing data [ ]	**Technically not feasible [ ]**	**Scientifically unjustified [X]**
Limited exposure [X]	**Other justification [ ]**	
Detailed justification:	The use pattern of acrolein would lead to negligible exposure to soil. The rate and route of degradation in soil has already been elucidated in studies on the estimation of the aerobic biotransformation rates for acrolein (Magnacide®H Herbicide, Magnacide®B Microbiocide) in soil (Section A7.2.1, Annex Point IIIA, VII.4., Ann. IIIA, XII.1.1.) and the soil adsorption coefficient for acrolein (Magnacide®Herbicide and Magnacide®B Microbiocide) study (Section A7.1.3, Annex Point IIIA, XII.2.2.) Therefore, in view of the low exposure potential in soil from use and the existing data further studies are considered not to be necessary	
Undertaking of intended data submission [ ]		
	Evaluation by Competent Authorities	
	Use separate "evaluation boxes" to provide transparency as to the comments and views submitted	
	EVALUATION BY RAPPORTEUR MEMBER STATE	
Date	*Give date of action*	
Evaluation of applicant's justification	*Discuss applicant's justification and, if applicable, deviating view*	
Conclusion	*Indicate whether applicant's justification is acceptable or not. If unacceptable because of the reasons discussed above, indicate which action will be required, e.g. submission of specific test/study data*	
Remarks		
	COMMENTS FROM OTHER MEMBER STATE *(specify)*	
Date	*Give date of comments submitted*	
Evaluation of applicant's justification	*Discuss if deviating from view of rapporteur member state*	
Conclusion	*Discuss if deviating from view of rapporteur member state*	
Remarks		

Section A7.2.2.4 Annex Point IIA7.2.2.4		Fate and behaviour in soil: anaerobic degradation in soil	
		1 REFERENCE	**Official use only**
1.1	**Reference**	Chou, T-W. & Spanggord, R.J. (1991) Estimation of the Anaerobic Biotransformation Rates for Acrolein (Magnacide®H Herbicide, Magnacide®B Biocide) in Soil-Water Mixture. SRI International. SRI Project No. 3562-4.	
1.2	**Data protection**	Yes	
1.2.1	Data owner	Baker Petrolite	
1.2.2	Criteria for data protection	Data on new a.s. for first entry to Annex I	
		2 GUIDELINES AND QUALITY ASSURANCE	
2.1	**Guideline study**	Yes FIFRA 162-2 and 162-3	X
2.2	**GLP**	No No GLP statement provided	X
2.3	**Deviations**	No	
		3 MATERIALS AND METHODS	
3.1	**Test material**	As given in Section 2	
3.1.1	Lot/Batch number	NN-481-76	
3.1.2	Specification	As given in Section 2 Deviating from specification given in section 2 as follows Radiolabelled at the 2 and 3 positions (acrolein-2,3-^{14}C)	
3.1.3	Purity	See 3.1.2	
3.1.4	Further relevant properties		X
3.1.5	Method of analysis		X
3.2	**Degradation products**	Degradation products tested: Yes	
3.2.1	Method of analysis for degradation products	At various time points, aliquots from the six flasks (two sterile and four non-sterile) were removed and placed in amber glass vials. The vials were centrifuged at 2500 rpm for 10 minutes and the acetonitrile (plus 1.2 ml water originally added) was carefully pipetted into a vial and capped. The aqueous supernatants were analysed by high-performance liquid chromatography (HPLC) using the following conditions: Instrument: Spectra-Physics Model 8000 Liquid Chromatograph Column: Regis Hi-Chrom ODS-II column, 4.6 x 250 mm Solvent: Water/Acetonitrile (80/20) Flow rate: 1.0 ml/minute Detectors: UV at 210 nm in series with a Raytest solid-state radioactivity detector	

Section A7.2.2.4 Annex Point IIA7.2.2.4		Fate and behaviour in soil: anaerobic degradation in soil	
		Quantitation was achieved using the external standard method relating peak area to parts per million (ppm) of acrolein injected as determined from standard calibration curves. Total radioactivity in the aqueous phase was determined by direct counting of a 100 µl in 10 ml of Aquasol scintillation counting liquid. The soil samples were oxidised using a Packard Model 306 Oxidizer where the sample is combusted and the ^{14}C-carbon is converted to ^{14}C-carbon dioxide and trapped. The trapped activity is counted in a scintillation counter.	
3.3	**Reference substance**	No	
3.3.1	Method of analysis for reference substance	Not applicable	
3.4	**Soil types**	See Table A7_2_2_4-1	
3.5	**Testing procedure**		
3.5.1	Test system	Soil biotransformation rate studies were performed in 125 ml Erlenmeyer flasks. Each flask was equipped with an internal carbon dioxide trap containing 10ml of a 0.2M potassium hydroxide solution, and a pressure relief valve to allow nitrogen to enter the flask through a sterilised filter when the flask was being sampled. Six flasks were prepared by weighing 6.0 g of Phoenix soil into three flasks and 6.0 g Menlo Park soil into the other three flasks. One flask containing each soil and 60 ml of Milli-Q water was autoclaved for one hour, then the water level was brought to 120 ml with sterilised water. To each non-sterile flask was added 120 ml of deionised water followed by 1.0 ml of a 0.5 ml/l filter sterilised resazurin solution as an oxidation-reduction indicator. The contents were thoroughly mixed with a stir-bar and the flasks were incubated at room temperature (20 ± 3°C) for 30 days. During the incubation, aerobic bacteria grew initially, consumed the dissolved oxygen, and reduced the water to an anaerobic condition. This effect was noted by a change in the resazurin dye which progressed from a blue-violet to pink to colourless solution. To accelerate the utilisation of oxygen in the Phoenix soil-water flasks, 10 ppm of Difco nutrient broth was added.	
3.5.2	Test solution and Test conditions	A stock solution of ^{14}C-acrolein in water was prepared by adding 0.37 ml of the test material solution to 29.6 ml of sterilised water. 2.0 ml of this solution was added to the sterile and non-sterile flasks while flushing with nitrogen, to yield a 4.2 ppm acrolein spike to the soil-water. The water-soil-containing flasks were capped to minimise volatilization and stirred with the magnetic-stir bar for 10 minutes. For sample analysis, 1.0 ml aliquots were removed by syringe, placed in a capped vial, and centrifuged at 2500 rpm for 10 minutes. Sampling and analysis were performed on Days 0, 2, 7, 14, 21, 28, 35, 42 and 56 after application.	
3.6	**Test performance**		
3.6.1	Identification of products	Products were identified by their co-chromatography with authentic standards or as derivatised products. Two derivatisation procedures were used. One procedure involved the conversion of aldehydes to their pentafluorophenylhydrazones by reaction with	

Section A7.2.2.4 Annex Point IIA7.2.2.4	Fate and behaviour in soil: anaerobic degradation in soil	
	pentafluorophenylhydrazine. The derivatives were then analysed by HPLC as described in section 3.2.1 with the exception that the gradient programme was used, starting from acetonitrile/water (20/80) for five minutes programmed to 100% acetonitrile in five minutes (six minute hold). The column was re-equilibrated for five minutes with the starting solvent composition. The components, 3-hydroxypropanal pentafluorophenylhydrazone and acrolein pentafluorophenylhydrazone eluted at 12.5 and 14.5 minutes respectively. To confirm, identifications were performed by gas chromatography/mass spectroscopy using a Ribermag R-10-10 GC/MS and a 30 m DB-5 fused silica capillary temperature programmed from 50 - 200°C	
3.6.2 Analysis of Data	The loss of acrolein from soil was assumed to a following a first-order reaction as shown in Equation 1: **Equation 1** $-d[A]/dt = k_b [A]$ Where [A] is the concentration of acrolein k_b is the first-order biotransformation rate constant t is time. Integration of equation 1 yields equation 2 **Equation 2** $\ln [A_o]/[A_t] = k_b t$ Where $[A_o]$ is the concentration of acrolein at time zero $[A_t]$ is the concentration at time t. Other loss processes (irreversible sorption, hydrolysis and volatilization) are occurring to acrolein on soil besides biotransformation. The half life of acrolein in soil due to biotransformation : $t½ = \ln 2/k_b$	
3.6.3 Screening test: Desorption	Not performed	
3.6.4 HPLC-method	According to OECD-HPLC-method: Yes	
	4 RESULTS	
4.1 Biotransformation Rate	Acrolein was found to be rapidly lost from both the sterile and non-sterile Phoenix and Menlo Park soil-water reaction flasks. Acrolein was completely gone from the aqueous phase within 14 days in both types of non-sterile soils. The sterile soil-water mixtures showed the presence of acrolein up to Day 56. The first-order rate constant for the Phoenix soil-water was averaged to 0.192/day. The first-order rate constant for the sterile control was 0.154/day. The first-order rate constant for the Menlo Park soil-water mixtures were averaged to be 0.239/day for the non-sterile soil-water, and 0.147/day for the sterile samples. The average half-life in the Phoenix soil was 3.6 days, while the half-life	

Section A7.2.2.4 Annex Point IIA7.2.2.4	Fate and behaviour in soil: anaerobic degradation in soil	
	in the sterile control was 4.5 days. In Menlo Park soil, the half-life was 2.9 days and half-life of the sterile control was 4.9 days. For both of the sterile soils, the average rate constant was calculated to be 0.151/day. The difference between the averaged non-sterile and sterile rate constants is 0.038/day in Phoenix soil-water and 0.092/day in Menlo Park soil-water from which an average anaerobic biotransformation half-life was 11 days.	
4.2 **Products**	Two products were identified; 1. 2-hydroxypropanal Acrylic acid – 2. 3-hydroxypropanal These products remained in the sterile controls with in equilibrium with acrolein up to Day 56. In the non-sterile samples, compound was transformed to 1,3-propanediol. Small amounts of 3-hydroxypropionic acid was also found. Carbon dioxide was identified as the final product resulting from acrolein biotransformation. This was continuously released between days 14 till the end of the study. The sterile controls showed minimal carbon dioxide production.	X
4.3 **Material balance**	In the sterile Menlo Park soil, the majority of the activity was found in the aqueous phase and potassium hydroxide trap. Approximately 4% of the activity was bound to the soil at the end of the study. In the non-sterile soil, the bound activity was slightly higher (6.7 - 6.9%) and the bound activity was being converted to carbon dioxide. Minimal activity was found bound to the Phoenix soil and the total recovery averaged 90%.	
	5 APPLICANT'S SUMMARY AND CONCLUSION	
5.1 **Materials and methods**	This study was conducted in accordance to FIFRA guidelines No. 162-2. Six flasks were prepared by weighing 6.0 g of Phoenix soil into three flasks and 6.0 g Menlo Park soil into the other three flasks. One flask containing each soil and 60 ml of Milli-Q water was autoclaved for one hour, then the water level was brought to 120 ml with sterilised water. To each non-sterile flask was added 120 ml of deionised water followed by 1.0 ml of a 0.5 ml/l filter sterilised resazurin solution as an oxidation-reduction indicator. The contents were thoroughly mixed with a stir-bar and the flasks were incubated at room temperature (20 ± 3°C) for 30 days. During the incubation, aerobic bacteria grew initially, consumed the dissolved oxygen, and reduced the water to an anaerobic condition. This effect was noted by a change in the resazurin dye which progressed from a blue-violet to pink to colourless solution. To accelerate the utilisation of oxygen in the phoenix soil-water flasks, 10 ppm of difco nutrient broth was added. To sterile and non-sterile flasks was added 2.0 ml of test material while flushing with nitrogen to yield a 4.2 ppm acrolein spike to the soil-water. The water-soil containing flasks were capped to minimise volatilization and stirred with the magnetic-stir bar for 10 minutes. For sample analysis, 1.0 ml aliquots were removed by syringe, placed in a capped vial, and centrifuged at 2500 rpm for 10 minutes.	

Section A7.2.2.4 Annex Point IIA7.2.2.4	Fate and behaviour in soil: anaerobic degradation in soil	
	Sampling and analysis was performed on Days 0, 2, 7, 14, 21, 28, 35, 42 and 56 after application.	
5.2 Results and discussion	Acrolein undergoes bio-transformation in anaerobic soil-water compartments. The half life was determined to be 2.9 and 3.6 days in Menlo Park and Phoenix soil-water mixtures. When corrected for sterile control, the half life was estimated to be 11 days. 3-hydroxypropanal is the hydrolytic product of acrolein, which is at it's maximum concentration after 7 days after which it is converted to 1,3-propandiol. This reaches maximum concentration after 14 days and is further transformed to 3-hydroxypropionic acid . Further oxidation possibly leads to malonyl derivatives (acid and aldehyde) and acetate. 1,3-propanediol and 3-hydroxypropionic acid are also readily biotransformed and are presumably converted to carbon dioxide with a half-life between 80 and 110 days. Acrolein products that are bound to soil are mineralised to carbon dioxide.	X
5.3 Conclusion	Biotransformation of acrolein and its abiotic transformation products will occur readily in an-aerobic soil-water eventually leading to carbon dioxide. Based on the rapid evolution of carbon dioxide, it appears that anaerobic soil-water microbes adapt easily to concentrations above any expected field exposure value. Thus, microbes will play an important role in the overall persistence of acrolein in anaerobic soil-water environments.	
5.3.1 Reliability	1	
5.3.2 Deficiencies	No	
	Evaluation by Competent Authorities	
	Use separate "evaluation boxes" to provide transparency as to the comments and views submitted	
	EVALUATION BY RAPPORTEUR MEMBER STATE	
Date	17/07/2007 The Applicant's version is acceptable, noting the following; **2.1** FIFRA guideline 162-2 was followed for this study. Guideline 162-3 refers to 'Anaerobic Aquatic Metabolism Studies' and is therefore non-applicable. **2.2** There is no certification of GLP (see remarks)	
Materials and Methods	The Applicant's version is considered acceptable, noting the following: **3.1.4** The UK CA believes that the water solubility figure should be given (237,628mg/l ± 2856 mg/l at 25°C). **3.1.5** The method of analysis should be stated (HPLC and Scintillation Counting).	

Section A7.2.2.4 Annex Point IIA7.2.2.4	Fate and behaviour in soil: anaerobic degradation in soil	
Results and discussion	The Applicant's version is considered acceptable, with the following additional comments; **4.2** The UK CA believes that the study summary is incorrect with respect to the following statement: *Two products were identified;* *1. 2-hydroxypropanal Acrylic acid* 2. *3-hydroxypropanal* Although this is a direct interpretation of what is stated in the study report, the UK CA believes that the report incorrectly states that one of the products is '2-*hydroxypropanal Acrylic acid*'. The two products identified where 3-hydroxypropanal and the hydrated 3-hydroxypropanal. Therefore, section 4.2 should read as follows: *Two products were identified;* *1. 3-hydroxypropanal* *2. hydrated 3-hydroxypropanal* **5.2** The UK CA suggest that the wording below is used: 3-hydroxypropanal is the hydrolytic product of acrolein, which is at it's maximum concentration (67.2 % AR) after 7 days, and is then converted to 1,3-propandiol, whis reaches maximum concentration (53.2 % AR) after 14 days and is further transformed to 3-hydroxypropionic acid, which has a maximum concentration of 51.3 % AR after 28 days . Further oxidation possibly leads to malonyl derivatives (acid and aldehyde) and acetate. Using zero order kinetics, it is estimated that complete mineralization to CO_2 will yield a half-life of 80 - 110 days. Acrolein products that are bound to soil are mineralised to carbon dioxide. The total recovery at termination of the study was approximately 90 %. This therefore illustrates that the potential maximum amount of bound residues remaining is $\leq$ 10 %.	
Conclusion	The Applicant's version is considered acceptable.	
Reliability	2	
Acceptability	Acceptable The reliability factor has been changed to 2 because there is no certificate of GLP. However, it should be noted that the study was started prior to 1989, which is the year in which GLP use begun, hence GLP certification may not have been readily available at this time. The UK CA believes that the data reported in the study are considered sufficiently robust for risk assessment.	
Remarks	All endpoints and data presented in the summary have been checked against the original study and are correct. The UK CA notes that the Applicant has included uncompleted tables within the study summary (A7_2_2_4-2, A7_2_2_4-3, and A7_2_2_4-4). This will not affect the reliability factor of the study.	

Section A7.2.2.4 **Annex Point IIA7.2.2.4**	**Fate and behaviour in soil: anaerobic degradation in soil**
	COMMENTS FROM ...
Date	*Give date of comments submitted*
Materials and Methods	*Discuss additional relevant discrepancies referring to the (sub)heading numbers and to applicant's summary and conclusion.* *Discuss if deviating from view of rapporteur member state*
Results and discussion	*Discuss if deviating from view of rapporteur member state*
Conclusion	*Discuss if deviating from view of rapporteur member state*
Reliability	*Discuss if deviating from view of rapporteur member state*
Acceptability	*Discuss if deviating from view of rapporteur member state*
Remarks	

Table A7_2_2_4-1:Classification and physico-chemical properties of soils used as adsorbents

	Soil 1	**Soil 2**
Soil identification	Phoenix	Menlo Park
Classification	Sandy loam	Loam
Location	S.32nd Street, Phoenix, Arizona, USA	S.32nd Street, Phoenix, Arizona, USA
Sand [%]	61.4	46.0
Silt [%]	24.6	31.8
Clay [%]	14.0	22.2
Organic matter [%]	0.4	4.0
pH (1:1 H_2O)	7.9	5.9
Cation exchange capacity (MEQ/100 g)	9.1	21.5

Table A7_2_2_4-2: Results of preliminary test:

Test substance	
Sample purity	
Weighed soil	
Volume of calcium chloride solution	
Nominal concentration of a.s. final solution	
Analytical concentration final of a.s. solution	
Concentration of the test solution (show calculation)	
Details of the analytical method used:	
Method	
Recovery rate	
Detection limit	

Table A7_2_2_4-3: Results of screening test - adsorption:

	Soil 1		Soil 2	
Concentration of test material [mg/l]				
After contact of....hours with soil				
Correction for blank with soil				
Correction for blank without soil				
Final corrected concentration [mg/l]				
Initial concentration of test solution [mg/l]				
Decrease in concentration [mg/l]				
Quantity adsorbed [µg]				
Quantity of soil [g of oven-dried equivalent]				
Quantity adsorbed [µg] per gram of soil				
Test material adsorbed [%]				
Temperature [°C]				
Volume of solution recovered after centrifugation [ml]				
Volume of solution not recovered [ml]				
Corresponding quantity of test substance [mg]				

Table A7_2_2_4-4: Results of screening test - desorption:

	Soil 1		Soil 2	
Temperature [°C]				
Concentration in combined washings [mg/l]				
Corresponding quantity of test material [mg]				
Quantity desorbed [µg]				
[%] of adsorbed test material, which is desorbed				
[%] of adsorbed test material, which is not desorbed				

Section A7.2.3 Annex Point IIIA.XII.1.2.-3	Adsorption and mobility in soil, further studies	
	JUSTIFICATION FOR NON-SUBMISSION OF DATA	**Official use only**
Other existing data [ ]	**Technically not feasible [ ]** **Scientifically unjustified [X]**	
Limited exposure [ ]	**Other justification [ ]**	
Detailed justification:	The use pattern of acrolein would lead to negligible exposure to soil. The mobility in soil has already been elucidated in studies on the estimation of the aerobic biotransformation rates for acrolein (Magnacide®H Herbicide, Magnacide®B Microbiocide) in soil (Section A7.2.1, Annex Point IIIA, VII.4., Ann. IIIA, XII.1.1.) and the soil adsorption coefficient for acrolein (Magnacide®Herbicide and Magnacide®B Microbiocide) study (Section A7.1.3, Annex Point IIIA, XII.2.2.) Therefore, in view of the low exposure potential in soil from use and the existing data further studies are considered not to be necessary	
Undertaking of intended data submission [ ]		
	Evaluation by Competent Authorities	
	Use separate "evaluation boxes" to provide transparency as to the comments and views submitted	
	EVALUATION BY RAPPORTEUR MEMBER STATE	
Date	18/05/2006	
Evaluation of applicant's justification	The Applicant's justification is acceptable.	
Conclusion	Acceptable	
Remarks		
	COMMENTS FROM OTHER MEMBER STATE *(specify)*	
Date	*Give date of comments submitted*	
Evaluation of applicant's justification	*Discuss if deviating from view of rapporteur member state*	
Conclusion	*Discuss if deviating from view of rapporteur member state*	
Remarks		

Section A7.2.3.1 **Annex Point IIIA XII.1.2**	**Adsorption and desorption accordance with the new test guideline EC C18 or the corresponding OECD 106 and, where relevant, adsorption and desorption of metabolites and degradation products**	
	JUSTIFICATION FOR NON-SUBMISSION OF DATA	**Official use only**
Other existing data [ ] **Limited exposure [X]**	**Technically not feasible [ ]** **Scientifically unjustified [X]** **Other justification [ ]**	
Detailed justification:	A full OECD study in 5 soils is not required as a determination of absorption in soil has been performed. See section IIIA7.1.3. The substance and product will be used in a marine environment only and therefore there will be no terrestrial exposure.	
Undertaking of intended data submission [ ]		
	Evaluation by Competent Authorities	
	Use separate "evaluation boxes" to provide transparency as to the comments and views submitted	
	EVALUATION BY RAPPORTEUR MEMBER STATE	
Date	18/05/2006	
Evaluation of applicant's justification	The Applicant's justification is acceptable.	
Conclusion	Acceptable	
Remarks		
	COMMENTS FROM OTHER MEMBER STATE *(specify)*	
Date	*Give date of comments submitted*	
Evaluation of applicant's justification	*Discuss if deviating from view of rapporteur member state*	
Conclusion	*Discuss if deviating from view of rapporteur member state*	
Remarks		

Section A7.3.1(1) Annex Point IIIA VII.5		Phototransformation in air including identity of transformation products	
		1 REFERENCE	Official use only
1.1	**Reference**	Haag, W.R. et al. (1988b) Estimation of Photolysis Rate Constants for Acrolein (Magnacide®H Herbicide and Magnacide®B Microbiocide) in the Environment, SRI International, SRI Project No. 3562-3.	
1.2	**Data protection**	Yes	
1.2.1	Data owner	Baker Petrolite	
1.2.2	Criteria for data protection	Data on new a.s. for first entry to Annex I	
		2 GUIDELINES AND QUALITY ASSURANCE	
2.1	**Guideline study**	Yes FR 796.3780 and Pesticide Assessment Guidelines, Subdivision N, 161-3	X
2.2	**GLP**	Yes	
2.3	**Deviations**	No	X
		3 METHOD	
3.1	**Test material**	As given in Section 2	
3.1.1	Lot/Batch number	NN-481-76	
3.1.2	Specification	As given in Section 2	
3.1.3	Purity	96.2 %	
3.1.4	Radiolabelling	Not used	
3.1.5	UV/VIS absorption spectra and absorbance value	Extinction coefficients were estimated relative to the maximum of 11,800 M^{-1} cm^{-1} at 210 nm using the respective attenuations	
3.1.6	Further relevant properties	None	
3.2	**Reference substance**	No	
3.2.1	Initial concentration of reference substance		
3.3	**Test solution**	See Table A7_3_1-1	
3.4	**Testing procedure**		
3.4.1	Test system	Sunlight irridation was performed in a 5 l Pyrex bulk equipped with a stopclock and a septum-capped side port. The bulb was purged with nitrogen gas at 100 ml/min for 30 minutes, then with synthetic air at 50 ml/min for 50 minutes. Acrolein (60 µg/l) and methylene chloride (57.7 µg/l) were added by injection to give final concentrations of 180 µM each. The bulb was clamped above a grey surface on the roof of the SRI Physical Sciences building in Menlo Park, California, USA and exposed for 11 cloudless days from 17 July 1987 to 27 July 1987. An identically	X

Section A7.3.1(1) Annex Point IIIA VII.5		Phototransformation in air including identity of transformation products	
		prepared bulb kept in the laboratory in the dark served as the control. The temperature was ambient, approximately 25 to 30°C during daylight. Analyses were performed at regular time intervals by removing a 10 µl sample (after three syringe rinses) through the septum using a pressure lock syringe and injecting into a Varian 3700 gas chromatograph equipped with a flame ionisation detector..	
3.4.2	Properties of light source	See Table A7_3_1-2	X
3.4.3	Determination of irradiance	A sunlight actinometer was used for kinetic studies. The solution contained 10 µM p-nitroacetophenone and 20 mM pyridine.	
3.4.4	Temperature	25 ± 5 °C	X
3.4.5	pH	7	
3.4.6	Duration of test	11 days	
3.4.7	Number of replicates	Not specified	
3.4.8	Sampling	Samples were taken at 0, 1.0, 3.7, 7.0, 8.1 (run 2 only) and 11.0 hours.	
3.4.9	Analytical methods	Analyses were performed at regular time intervals by removing a 10 µl sample (after three syringe rinses) through the septum using a pressure lock syringe and injecting into a Varian 3700 gas chromatograph equipped with a flame ionisation detector. Conditions were as follows: Column: 0.32 mm i.d. x 30 m DB-5 Nitrogen flow rate: 0.5 ml/min Air/hydrogen (2:1) flow rate): 30 ml/min A gas phase UV spectrum of acrolein was obtained by injection of 0.1 µl of acrolein from a 1.0 µl syringe into a 28.3 ml, 10 cm quartz cell (acrolein = 0.96 torr) and recording the spectrum on an HP 8450 diode array sprectrophotometer.	
3.5	**Transformation products**	Yes	
3.5.1	Method of analysis for transformation products	3-hydroxypropanal was analysed by HPLC following derivatisation with PFPH.	
		4 RESULTS	
4.1	**Screening test**	Not performed	
4.2	**Actinometer data**		
4.3	**Controls**		
4.4	**Photolysis data**		
4.4.1	Concentration values		
4.4.2	Mass balance		
4.4.3	k^c_p	0.090 d^{-1}	

Section A7.3.1(1) Annex Point IIIA VII.5	Phototransformation in air including identity of transformation products	
4.4.4 Kinetic order		
4.4.5 k^c_p / k^a_p		
4.4.6 Reaction quantum yield (ϕ^c_E)		
4.4.7 k_{pE}		
4.4.8 Half-life ($t_{1/2E}$)	7.7 days	
	5 APPLICANT'S SUMMARY AND CONCLUSION	
5.1 Materials and methods	The study was performed according to the protocols in Federal Register 796.3780 and Pesticide Assessment Guidelines, Subdivision N, 161-3. Sunlight irradiations were performed on the acrolein/methylene chloride samples on 11 consecutive cloudless days. Sampling occurred at 0, 1.0, 3.7, 7.0, 8.1 (run 2 only) and 11.0 hours. Photolyses were run at ambient temperature (25 ± 5°C) During analysis, acrolein levels were determined by gas chromatography, with a gas UV spectrum of acrolein obtained by a HP 8450 diode array spectrophotometer.	X
5.2 Results and discussion	There was a small, rapid initial loss, but it was not thought to be due to direct photolysis. Possible explanations include incomplete mixing when the zero time point was taken, adsorption of acrolein onto the walls of the bulb, or incomplete removal by purging with synthetic air of nitrogen oxides and other hydroxide radical precursors, which were rapidly consumed in the initial part of the reaction. Acrolein may be lost from the troposphere by sensitised photo-oxidation. The most important photo-oxidant in the troposphere is the hydroxy radical, present in average concentrations of approximately 5E+5 molecules/cm^3. Using a rate constant of 1.9E-11 cm^3/molecule/s for reaction of acrolein with the hydroxy radical, a first order rate constant of 1.9E-05 s^{-1} or a half life of 29 hours for tropospheric consumption of acrolein by hydroxy radicals, which is nearly 10 times faster than the measured direct photolysis rate. Ozone may oxidise acrolein. Assuming an average ozone concentration of 1E+22 molecules/cm^3 and a rate constant of 2.8E-19 cm^3/molecule/s for acrolein, an ozoneation rate constant of 2.8E-07 s^{-1} or half life of 41 days is calculated. Therefore, ozone reactions will be negligible and hydroxy radical reactions will control the tropospheric transformation rate of acrolein. The report states that the products from direct photolysis of acrolein under atmospheric conditions are carbon monoxide (75%), carbon dioxide (29%), glyoxal (31%), ethylene (27%), methanol (5%), formaldehyde (6%) and methane (1%). Hydroxy attack on acrolein will occur primarily at the aldehydic hydrogen, probably yielding acrylic acid after several steps. Acrolin and acrylic acid can both add hydroxy radicals to the double bond to form a variety of polar products.	X
5.2.1 k^c_p		
5.2.2 K_{pE}	0.090 d^{-1}	
5.2.3 φ^c_E		
5.2.4 $t_{1/2E}$	7.7 days	

Section A7.3.1(1) Annex Point IIIA VII.5	Phototransformation in air including identity of transformation products	
5.3 Conclusion	The observed rate constant for the gas phase photolysis of acrolein was measured at 0.063 d^{-1} yielding a half-life of 10.9 days. The calculated rate constant was 0.090 d^{-1} or a half-life of 7.7 days. Estimation of half-lives from other atmospheric oxidation processes indicated reactions with hydroxy radicals (HO) would be rapid (half-life = 29 hours) and reactions with ozone much slower. (Half-life = 41 days).	
5.3.1 Reliability	2	
5.3.2 Deficiencies	Yes The report states that the products from direct photolysis of acrolein under atmospheric conditions are carbon monoxide (75%), carbon dioxide (29%), glyoxal (31%), ethylene (27%), methanol (5%), formaldehyde (6%) and methane (1%). These values added together give a total of 174 %. Unfortunately, it is not readily possible to explain the origin of the disproportionate percentage results cited by Haag *et al*. These results are claimed to originate from an EPA report by Gardner *et al* (Gardner, Sperry and Calver, Primary Photochemical Processes of Acrolein, EPA, 1986). Peter Fisk Associates (PFA), experts in Environmental Chemistry have reviewed both reports and although they have explored some realistic conversions, there is no obvious way that these percentages could have been calculated from the results that are presented in the Gardner *et al* report. PFA's comments have been provided as an appendix to this robust summary and a robust summary has been written on the EPA report (see Document IIIA Section 7.3.1(2)). The disproportionate percentages do not affect the validity of the report, since the general findings are supported by the Gardner *et al* report. This report states that the order of abundance of phototransformation products of acrolein are: Carbon monoxide > ethylene > formaldehyde ≈ hydrogen > glyoxal > carbon dioxide > methanol ≈ methane. The report also states that degradation of acrolein via direct photolysis is much slower than degradation via reaction with hydroxyl radicals (half lives of > 5 days and 14.6 hours, respectively). Hence indirect photolysis is the major and more important route of degradation.	
	Evaluation by Competent Authorities	
	Use separate "evaluation boxes" to provide transparency as to the comments and views submitted	
	EVALUATION BY RAPPORTEUR MEMBER STATE	
Date	13/07/2007	

Section A7.3.1(1) Annex Point IIIA VII.5	Phototransformation in air including identity of transformation products
Materials and Methods	The Applicant's version is considered acceptable with the following exceptions: **2.1** The guideline stated by the applicant, *Pesticide Assessment Guidelines, Subdivision N, 161-3,* is for 'Photodegradation Studies in Soil'. The applicant has actually followed the correct guideline, '161-4: Photodegradation studies in Air'. **2.2** No data on hours of daylight, See point **3.4.2.** **3.4.1** The units used for Acrolein and Methylene Chloride, $\mu g\ l^{-1}$, are incorrect. The study states that the units are µl. This will not affect the endpoint from the study. **3.4.2 Table A7_3_1-2: Description of test system.** Hours of daylight are not included in the table. This is a requirement of guideline 161-4. This will not affect the endpoint from the study. **3.4.4** The guideline, 161-4, states that the temperature should be maintained as closely to 30 °C as possible. This will not affect the endpoint from the study. **5.1** see point **2.1** **5.2** The figure given in the summary for average ozone concentration is incorrect. The study states this figure should be 1×10^{12}. This will not affect the endpoint from the study.
Results and discussion	The Applicant's version is considered to be acceptable.
Conclusion	The Applicant's version is considered to be acceptable.
Reliability	2
Acceptability	Acceptable
Remarks	All endpoints and data presented in the summary have been checked against the original study and are correct (with the exceptions of those noted above).
	COMMENTS FROM ... *(specify)*
Date	*Give date of comments submitted*
Materials and Methods	*Discuss additional relevant discrepancies referring to the (sub)heading numbers and to applicant's summary and conclusion.* *Discuss if deviating from view of rapporteur member state*
Results and discussion	*Discuss if deviating from view of rapporteur member state*
Conclusion	*Discuss if deviating from view of rapporteur member state*
Reliability	*Discuss if deviating from view of rapporteur member state*
Acceptability	*Discuss if deviating from view of rapporteur member state*
Remarks	

Table A7_3_1-1: Description of test solution and controls

Criteria	Details
Purity of water	Unbuffered Milli-Q water
Preparation of test chemical solution	Solutions of 10 ppm acrolein in 10 mg/l humic acid prepared by diluting 0.5 ml of 1000 ppm acrolein stock, 5 ml of 100 mg/l humic acid stock and 1.0 ml of 0.5M pH 7 phosphate buffer to 50 ml.
Test concentrations (mg a.s./l)	Initial concentration: 10 ppm acrolein.
Temperature (°C)	Ambient 25ºC ± 5ºC
Preparation of a.s. solution	Not applicable
Controls	Identical to test solution, but kept in the laboratory in the dark
Identity and concentration of co-solvent	No co-solvent used

Table A7_3_1-2: Description of test system

Criteria	Details
Laboratory equipment	5 l Pyrex bulb with stopcock and septum-capped side port. GC: Varian 3700 equipped with flame ionisation detector Spectrometer: HP 8450 diode array spectrophotometer *Give details on the type and geometry of the reaction vessels (test tubes, material, size, type of absorption cell, pathlength); describe applicability in relationship to the applied wavelength.* *Report the name and the model of the spectrometer used.*
Test apparatus	*e.g. sunlight actinometer; describe details*
Properties of artificial light source:	No artificial light source used.
Properties of natural sunlight:	Natural sunlight used
Latitude	40ºN
Hours of daylight	Not stated
Time of year	Summer (17 - 27 July 1987)
Light intensity	Not stated
Solar irradiance (L_λ)	Not stated

Section A7.3.1(2) Annex Point IIIA VII.5		Phototransformation in air including identity of transformation products	
		1 REFERENCE	Official use only
1.1	**Reference**	Gardner, E.P., Sperry, P.D. and Calvert, J.G. (1986). The Primary Photochemical Processes of Acrolein. EPA Report EPA/600/3-86/005. US EPA Research, Triangle Park, NC. 93 pp.	
1.2	**Data protection**	No. Report marked Unclassified: Release to Public	
1.2.1	Data owner	N/A	
1.2.2	Criteria for data protection	No data protection claimed	
		2 GUIDELINES AND QUALITY ASSURANCE	
2.1	**Guideline study**	Yes No formalised EU standard guideline is available. Methods and experimental equipment used were largely compliant with OECD monograph 61 (1993) section 3.4: Methods to Determine the Rate of Direct Photo-transformation. There are some deviations (see 5.3.2) and some aspects of the OECD method, if carried out in this study, are not reported (e.g. preliminary experiments across a range of time periods).	
2.2	**GLP**	No	
2.3	**Deviations**	Yes See 5.3.2	
		3 METHOD	
3.1	**Test material**	Acrolein	
3.1.1	Lot/Batch number	Not reported.	
3.1.2	Specification	Acrolein was obtained from Sigma Aldrich	
3.1.3	Purity	Acrolein as obtained: 97% pure in water; 200 ppm hydroquinone present Sample was further purified prior to the experiment; final purity estimated as 99.9% (refer to table A7_3_1-1)	
3.1.4	Radiolabelling	None	
3.1.5	UV/VIS absorption spectra and absorbance value	Absorbance at 313 nm. At this wavelength, in the test system used, only acrolein is absorbing. *Please see figure 1 for the UV absorption spectrum of acrolein.*	
3.1.6	Further relevant properties	None	
3.2	**Reference substance**	None	

Section A7.3.1(2) Annex Point IIIA VII.5		Phototransformation in air including identity of transformation products	
3.2.1	Initial concentration of reference substance	N/A	
3.3	**Test atmosphere**	See Table A7_3_1-1	
3.4	**Testing procedure**		
3.4.1	Test system	See Table A7_3_1-2	
3.4.2	Properties of light source	See Table A7_3_1-2	
3.4.3	Determination of irradiance	Light exiting the reaction cell passes into a photomultiplier tube (model 8575 RCA), with narrow band and neutral density filters, then into a Hewlett Packard 5201L scaler timer, digital pulse height analyser to obtain a measure of integrated light intensity.	
3.4.4	Temperature	24.08°C (run 7F) 22.3 – 25.8°C across 11 experimental runs	
3.4.5	Duration of test	Run time 1620 minutes = 27 hours (Run #7F). 1620 – 2770 minutes across 11 experimental runs	
3.4.6	Number of replicates	Eleven experimental runs in total. Quantum yields are presented for all runs but results discussed in the report relate only to one run (7F).	
3.4.7	Sampling	After photolysis, the reaction mixture flows into a reservoir/sample chamber, which incorporates a Dewar trap. The mixture passes into a sample loop.	
3.4.8	Analytical methods	From the sample loop the products are passed via Carle valves for analysis using a gas chromatograph fitted with flame ionisation detector (GC-FID) and thermal conductivity detector (GC-TCD). GC-mass spectrometry was used for primary identification of unknown products.	
3.5	**Transformation products**	Yes	

Section A7.3.1(2) Annex Point IIIA VII.5	Phototransformation in air including identity of transformation products	
3.5.1 Method of analysis for transformation products	Eight transformation products were identified by GC-MS. These are identified in Table A7_3_1-3, in which CAS numbers and full chemical names are presented, together with product-specific normalised mean molar ratios and other results. The report clearly states the finding that the order of abundance of phototransformation products of acrolein are: CO (Carbon monoxide) > C_2H_4 (Ethylene) > HCHO (Formaldehyde) ≈ H_2 (Hydrogen) > HCOCHO (Glyoxal) > CO_2 (Carbon dioxide) > CH_3OH (Methanol) ≈ CH_4 (Methane) Trace amounts of acetaldehyde, acetylene and acetic acid were also detected. *Notes:* *It is not made clear how 'abundance' has been calculated and this sequence does not correlate exactly with molar ratios/ number of molecules or the equivalent by weight or the quantum yields.* *There is very extensive reporting in this source of transformation mechanisms occurring at 313 nm. Over 20 separate reaction mechanisms are defined. It is not necessary to reproduce these here.*	
	4 RESULTS	
4.1 Screening test	Not reported	
4.2 Actinometer data	Two actinometers used, azomethane ($CH_3CN{=}NCH_3$) and acetone (O_2-free). Products are N_2 and CO respectively. Actinometer data are not presented in report. It is reported that the data indicate accuracy to within 10% and reproducibility better than ± 5% for the acrolein experiment.	
4.3 Controls	None	
4.4 Photolysis data		
4.4.1 Concentration values	Molar ratios of the products are presented in Table A7_3_1_3.	
4.4.2 Mass balance	As shown in Table A7_3_1_3, a mass balance (based on carbon atoms) of 2.69 moles C in products : 3.00 moles C in acrolein lost in the test system is achieved. This is equivalent to 90%, not including non-carbon products (hydrogen, water). The transformation processes and products are discussed in detail in the report, though this is not reproduced here. The small quantum yield of acrolein loss indicates efficient deactivation processes occurring. This is thought to be due to collisional transfer of vibrational energy to oxygen.	
4.4.3 k^c_p	Many pathways of decomposition are identified in the report and no single overall value of k^c is defined. It is of interest to consider the varying values of the first-order rate coefficient (J) presented in the report. J varies in accordance with solar zenith angle from 2.8E-06 s^{-1} at 0°, 2.3E-06 s^{-1} at 40°, to 0.08E-06 s^{-1} at 86°	

Section A7.3.1(2) Annex Point IIIA VII.5	Phototransformation in air including identity of transformation products	
4.4.4 Kinetic order	First order	
4.4.5 k^c_p / k^a_p	See section 4.4.3	
4.4.6 Reaction quantum yield (ϕ^c_E)	Quantum yields are reported for specific products. These results are presented in Table A7_3_1_3. The perfect quantum yield would be 1. In this study, quantum yields are derived for loss of acrolein and also generation of products. The sum of the yields for products is more than the yield from loss of acrolein because they are smaller molecules resulting from fragmentation. Quantum yields are shown in the study to be strongly affected by pressure, with much lower quantum yields at higher pressures. This indicates that reaction will be fastest at higher altitudes.	
4.4.7 k_{pE}	See section 4.4.3	
4.4.8 Half-life ($t_{1/2E}$)	Half-life for direct photolysis under atmospheric conditions, is reported in this study as >5 days. *Note:* *The authors point out in the concluding discussions that photodegradation by hydroxyl radicals will be a much more significant degradation process for acrolein than direct photolysis. A half-life for the hydroxyl radical process of 14.6 hours is reported.*	
4.5 Transformation products results	See Table A7_3_1-3 for transformation products, abundance data and quantum yields.	
	5 APPLICANT'S SUMMARY AND CONCLUSION	
5.1 Materials and methods	Direct photolysis of acrolein was studied. The study used a highly purified sample of acrolein (99.9% pure), a wavelength 313 nm, in a synthetic atmosphere comprising ca. 20% O_2 and 80% N_2. The test system comprised a vacuum line connected to the reaction cell, with direct outflow to a Varian model 2700 gas chromatograph. The vacuum line was comprised of five sections: storage, high vacuum/reference, measurement, calibration/mixture preparation, and distillation. Light passed from a UV light source (high pressure mercury arc lamp), via shutter and monochromator, through a window into a reaction cell. The reaction cell was connected to the vacuum system and featured photomultiplier tube, sampling reservoir, gas piston and outlet to GC analysis. Detection/analysis is by a gas chromatograph equipped with flame ionisation detector and thermal conductivity detector. It is reported that actinometer data indicate accuracy to within 10% and reproducibility better than ± 5% for the acrolein experiment.	

Section A7.3.1(2) Annex Point IIIA VII.5		Phototransformation in air including identity of transformation products	
5.2	**Results and discussion**	Eight transformation products were identified by GC-MS. The report clearly states the finding that the order of abundance of phototransformation products of acrolein are: CO (Carbon monoxide) > C_2H_4 (Ethylene) > HCHO (Formaldehyde) ≈ H_2 (Hydrogen) > HCOCHO (Glyoxal) > CO_2 (Carbon dioxide) > CH_3OH (Methanol) ≈ CH_4 (Methane) Trace amounts of acetaldehyde, acetylene and acetic acid were also detected. *Notes:* *It is not made clear how 'abundance' has been calculated and this sequence does not correlate exactly with molar ratios/ number of molecules or the equivalent by weight or the quantum yields.* *There is very extensive reporting in this source of transformation mechanisms occurring at 313 nm. Over 20 separate reaction mechanisms are defined. It is not necessary to reproduce these here.*	
5.2.1	k^c_p	Many pathways of decomposition are identified in the report and no single overall value of k^c is defined.	
5.2.2	K_{pE}	See section 5.2.1	
5.2.3	φ^c_E	Quantum yields are reported for specific products. These results are presented in Table A7_3_1_3. Quantum yields are shown in the study to be strongly affected by pressure, with much lower quantum yields at higher pressures. This indicates that reaction will be fastest at higher altitudes.	
5.2.4	$t_{1/2E}$	Half-life for direct photolysis under atmospheric conditions, is reported in this study as >5 days. *Note:* *The authors point out in the concluding discussions that photodegradation by hydroxyl radicals will be a much more significant degradation process for acrolein than direct photolysis. A half-life for the hydroxyl radical process of 14.6 hours is reported.*	
5.3	**Conclusion**	The authors' conclusions with regard to half-life are accepted.	
5.3.1	Reliability	(2) Study conducted in accordance with generally accepted scientific principles, possibly with incomplete reporting or methodological deficiencies, which do not affect the quality of relevant results	
5.3.2	Deficiencies	Yes Only one absorbing frequency was used in the test. OECD Monograph 61 recommends the use of two separate frequencies/wavelengths in separate tests to ensure the quantum yield is not frequency-dependent. The report acknowledges this as a potential weakness but indicates that it is not improbable that the results will be independent of wavelength. The high level of accuracy and reproducibility of the results means that the result is still reliable and useful in itself.	

Section A7.3.1(2) Annex Point IIIA VII.5	Phototransformation in air including identity of transformation products	
	Evaluation by Competent Authorities	
	Use separate "evaluation boxes" to provide transparency as to the comments and views submitted	

	EVALUATION BY RAPPORTEUR MEMBER STATE
Date	16/07/2007
Materials and Methods	The Applicant's version is considered acceptable.
Results and discussion	The Applicant's version is considered acceptable.
Conclusion	The Applicant's version is considered acceptable.
Reliability	3 See remarks section below
Acceptability	The Applicant's version is considered acceptable.
Remarks	The UK CA believes that the study and summary are acceptable as supporting evidence only as although the degradation products have been identified there is no quantification of them. Therefore the reliability factor has been reduced to 3. The study was not carried out to a specific guideline, but did follow an OECD Environmental Monograph 61 and is scientifically justified. The study is used as supporting evidence to Doc IIIA, A7.3.1 (1), with respect to the transformation products of acrolein during photolysis in air. The study summarised in Doc IIIA, A7.3.1 (1) states an acrolein half-life of 10.9 d, under experimental conditions. This study supports the transformation pathway only and therefore, for the environmental risk assessment, a full evaluation is not required.
	COMMENTS FROM ... *(specify)*
Date	*Give date of comments submitted*
Materials and Methods	*Discuss additional relevant discrepancies referring to the (sub)heading numbers and to applicant's summary and conclusion.* *Discuss if deviating from view of rapporteur member state*
Results and discussion	*Discuss if deviating from view of rapporteur member state*
Conclusion	*Discuss if deviating from view of rapporteur member state*
Reliability	*Discuss if deviating from view of rapporteur member state*
Acceptability	*Discuss if deviating from view of rapporteur member state*
Remarks	

Figure 1: UV absorption spectrum of acrolein

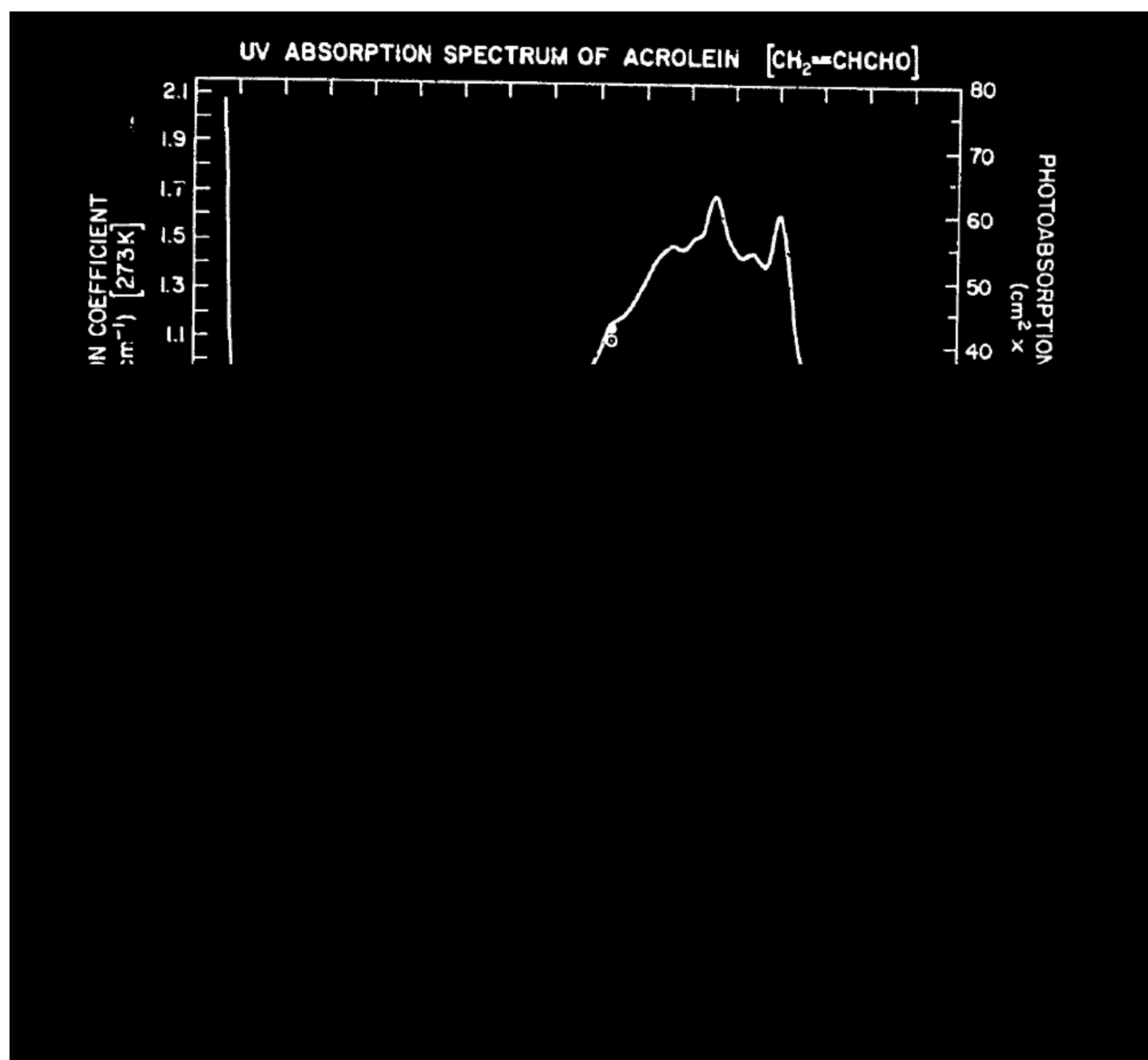


Table A7_3_1-1: Description of test atmosphere and controls

Criteria	**Details**
Purity of atmosphere	Oxygen and nitrogen obtained from Linde (Union Carbide Corp.) at 99.99% and 99.998% purity respectively.
Preparation of test chemicals	Acrolein purified by repeat distillation on the vacuum line and further purification by GC. Aliquots analysed by FID-GC (Porapak P/Q) showed no impurity detected. Minimum purity estimated 99.9%
Test concentrations (mg a.s./m^3)	1.39% acrolein in synthetic air (% by volume or weight not stated)
Temperature (°C)	Temperatures 22.3-25.8°C across 11 experimental runs
Pressure (Pa)	For all experimental runs, acrolein was tested at a pressure of 0.355 Torr (ca. 50 Pa) acrolein in a synthetic air, comprising ca. 20% O_2 and 80% N_2 The main experiment (Run 7F) conducted at 25.607 Torr (3414 Pa).
Preparation of a.s. test atmosphere	Atmosphere preparation not described in report.
Controls	None.
Actinometer	Two actinometers used, azomethane ($CH_3CN{=}NCH_3$) and acetone (O_2-free). Products are N_2 and CO respectively. Actinometer data are not presented in report. It is reported that the data indicate accuracy to within 10% and reproducibility better than ± 5% for the acrolein experiment.
Internal standard	Argon was used as internal standard, to establish normalised molar ratios of products. Mole fraction Argon in run 7F: 1.3982E-03

Table A7_3_1-2: Description of test system

Criteria	Details
Laboratory equipment	The internal optical path of the reaction cell was 155.8 cm with Suprasil windows fitted at the two ends. The windows were fitted so as to protrude inside the reaction cell, precluding any temperature disparity between the windows and the interior.
Test apparatus	The test system comprised a vacuum line connected to the reaction cell, with direct outflow to a Varian model 2700 gas chromatograph. The vacuum line was comprised of five sections: storage, high vacuum/reference, measurement, calibration/mixture preparation, distillation. Light passed from a UV light source (see below), via shutter and monochromator, through a window into a reaction cell. The reaction cell was connected to the vacuum system and featured photomultiplier tube, sampling reservoir, gas piston and outlet to GC analysis. The sample chamber was sealed from the reaction cell and its contents cryogenically fractionated and/or expanded into the gas piston, a spiral tube 118 cm long and 2.5 cm in diameter. Helium gas at greater than 1 atmosphere pressure was introduced and the sample is compressed into a 'plug' which enters the sample loop. The sample loop was re-evacuated using Carle sampling valves, controlled by Hewlett Packard 3390A computer/recorder. Detection/analysis was by gas chromatography equipped with flame ionisation detector and thermal conductivity detector. The carrier gas is Helium (99.99% pure). Column conditions are described in the report but it is not necessary to reproduce the details here.
Properties of artificial light source:	High pressure mercury arc lamp (OSRAM HBO 500 W/2) enclosed in Oriel C-60-51 lamp housing with quartz collimating lens. A narrow band interference filter (313 nm) enclosed in metal housing is introduced into the optical train to isolate initiating wavelength. Alternatively a Jarrell-Ash grating monochromator is inserted between the lamp housing and photolysis cell. A spectrum of the mercury arc lamp taken using a Varian/Cary 219 grating spectrophotometer is presented in the report. This is not reproduced here.

Table A7_3_1_3: Specification of transformation products, abundance data and quantum yields

CAS-Number	**CAS and/or IUPAC Chemical Name(s)**	**Normalised mean molar ratio**	**Number of molecules** from normalised mean molar ratio	**Molar ratios** normalised wrt. acrolein lost [1]	**Molar ratios** in terms of carbon atoms, normalised wrt. acrolein lost [1]	**Quantum yields**
630-08-0	Carbon Monoxide (CO)	1.630	8.936 E+18	**0.857**	0.857	0.0674
124-38-9	Carbon dioxide (CO_2)	0.244	1.338 E+18	**0.128**	0.128	0.0101
74-85-1	Ethylene *or* Ethene (C_2H_4)	1.260	6.908 E+18	**0.663**	1.326	0.0521
50-00-0	Formaldehyde *or* Methanal (HCHO)	0.3417	1.873 E+18	**0.180**	0.180	0.0141
7732-18-5	Water (HOH)	1.494	8.190 E+18	**0.786**	-	0.0618
67-56-1	Methanol (CH_3OH)	0.1011	5.543 E+17	**0.053**	0.053	0.00418
107-22-2	Glyoxal *or* 1,2-ethanedione (HCOCHO)	0.1357	7.439 E+17	**0.071**	0.143	0.00561
1333-74-0	Hydrogen (H_2)	0.2156	1.182 E+18	**0.113**	-	0.00891
	Acrolein (loss)	1.901	1.042 E+19	**1.000**	3.000	0.0786
	Argon	1.0				

Note:

1 – Product molar ratios normalised with respect to Acrolein loss: figures calculated by reviewer. Normalised mean molar ratios, number of molecules and quantum yield figures copied directly from Gardner *et al.*, 1986.

Section A7.3.2 **Annex Point IIIA XII.3**	**Fate and behaviour in air, further studies**	
	JUSTIFICATION FOR NON-SUBMISSION OF DATA	**Official use only**
Other existing data [ ] **Limited exposure [X]**	**Technically not feasible [ ]** **Scientifically unjustified [X]** **Other justification [ ]**	X
Detailed justification:	Acrolein is a highly volatile active substance (VP = 31920 Pa at 25°C) and undergoes volatilisation readily in water (A7.2.1) and therefore would be released to air under general use conditions. However, the active substance is applied via a closed system from sealed containers. If there was any release to the environment it would be via the aqueous environment where the substance undergoes rapid degradation by physico-chemical processes including rapid volatilisation (A7.2.1) and photodegradation (A7.1.1.1.2) and microbial degradation in water (anaerobic and aerobic freshwater-sediment radio-labelled studies, A7.1.2.1.1 and A7.1.2.1.2) transforming the active substance to CO2. The application system and containers are neutralised by purging with nitrogen gas followed by flushing of the system with methanol before opening to prevent vapour release (A2.10.1.2 Confidential information). The use pattern would lead to negligible exposure to air, therefore it is considered that studies in addition to the estimation of photolysis rate in air and the identification of the degradation products (Section A7.3.1, Annex Point IIIA, VII.5), are not necessary.	
Undertaking of intended data submission [ ]		
	Evaluation by Competent Authorities	
	Use separate "evaluation boxes" to provide transparency as to the comments and views submitted	
	EVALUATION BY RAPPORTEUR MEMBER STATE	
Date	19/05/2006	
Evaluation of applicant's justification	The Applicant's version is acceptable noting the following; **X**: The UKCA considers the justification to be acceptable due to limited exposure only. It is not considered to be scientifically unjustified. This issue is addressed in Doc IIC.	
Conclusion	Acceptable	
Remarks		
	COMMENTS FROM OTHER MEMBER STATE *(specify)*	
Date	*Give date of comments submitted*	
Evaluation of applicant's justification	*Discuss if deviating from view of rapporteur member state*	
Conclusion	*Discuss if deviating from view of rapporteur member state*	

Section A7.3.2 Annex Point IIIA XII.3	Fate and behaviour in air, further studies
Remarks	