

Aerobic Transformation of a Biocide in an Aquatic Marine Sediment System at 9°C

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INTRODUCTION

A modified OECD 308 study was performed at a constant 9°C for 90 days to determine the amount and rate of degradation of a biocide at the more environmentally relevant temperature of 9°C than the OECD 308 guideline temperature of 20°C.

AIMS AND OBJECTIVES

- Dose vessels either into the water phase or the sediment phase to monitor if there were any differences in degradation
- Kinetics analysis was performed on parent biocide in test system
- Non-extractable residue (NER) analysis was performed on all sediment samples to determine if the residues were Type I NER (sequestered, entrapped NER), Type II NER (covalently bound NER) or Type III NER (biogenic NER).

MATERIALS AND METHODS

This study had the following adaptations and enhancements from a standard OECD 308 to establish if degradation was altered:

- The study was performed at $9 \pm 2^\circ\text{C}$ in a marine sediment and water for 90 days
- The test substance was radiolabelled in two positions to enable tracking of different metabolites
- The seawater had mineral media added (following the OECD TG 306)
- Vessels were dosed either into the water phase or the sediment phase to monitor if there were any differences in degradation
- Sediment was not sieved to ensure optimal viability at study initiation
- Lower water:sediment ratio (1:1.6) to minimise movement of test substance between water and sediment

RESULTS AND KEY FINDINGS

The biocide showed the potential to biodegrade under the test conditions of $9 \pm 2^\circ\text{C}$.

The percent of applied radioactivity (AR) present as parent substance in the water and sediment on day 90 ranged from 22-27% for both radiolabels of the biocide dosed into either the water or sediment phase: dosing into either water or sediment phase gave similar results (Table 2).

Very low levels of mineralisation were observed under these conditions ranging from 1-3% of the AR.

The percentage of AR present in the sediment ranged from 77-99%; further NER analysis separated the AR as follows (Table 1 and Fig 1):

Non-extractable residue (NER) analysis	Extraction method	% of AR
Readily desorbable extracts	Aqueous extractions	< 2
Desorbable extracts	Organic solvent-water mixtures	30-41
Slowly desorbable extracts	Accelerated solvent extraction (ASE)	40-51
Type I NER, sequestered, entrapped NER	Silylation	< 1
Type II NER, covalently bound NER	Combustion	4-14
Type III NER, bioNER	Amino acid extraction	< 1

Single first order (SFO) kinetic analysis of the entire test system for both radiolabels of the biocide dosed into either the water or sediment phase gave DT_{50} of 32.1 - 34.4 days for the biocide (Table 3).

Biocide label 1 or 2	Phase dosed	Biocide (% of AR)				Metabolites (% of AR)			
		Day				Day			
		0	28	56	90	0	28	56	90
Label 1	Water	100	41	34	26	0.0	2.5	5.1	3.4
Label 2	Water	100	39	33	27	0.0	2.2	5.1	5.1
Label 1	Sed	100	38	35	22	0.0	2.2	4.6	4.4
Label 2	Sed	100	41	32	27	0.0	3.3	5.2	3.5

Table 2. Biocide & metabolites in test system measured by radio-TLC in test system over time (day 0 values nominal)

Biocide label 1 or 2	Phase dosed	K (degradation rate, per day)	DT_{50} (days)	DT_{90} (days)	R^2
Label 1	Water	0.0201	34.4	114	0.9129
Label 2	Water	0.0207	33.5	111	0.8999
Label 1	Sed	0.0216	32.1	107	0.9155
Label 2	Sed	0.0205	33.8	112	0.9086

Table 3. Kinetics calculated using nominal 100% at day 0 (SFO) Ref 3

Vessel	Biocide label 1 or 2	Phase dosed	Day	Sediment Extractable residues			Non-extractable residues			Total in sed (%)	Volatile & NaOH traps (%)	Total (%)	
				Overlying water (%)	Readily desorbable extracts (%)	Desorbable extracts (%)	ASE Extracts (%)	Type I (silylation) (%)	Type II (%)				Type III (bioNER) (%)
1	Label 1	Water	28	11.6	1.4	35.9	40.2	0.7	4.0	0.2	82.2	0.1	94
2	Label 2	Water		12.2	1.5	33.2	50.9	0.5	8.8	0.1	94.9	0.7	108
3	Label 1	Sed		8.0	1.3	34.6	42.1	0.3	10.7	0.1	89.1	0.1	97
4	Label 2	Sed		9.2	1.4	38.2	44.7	0.5	7.7	0.1	92.5	0.8	103
5	Label 1	Water	56	7.2	1.6	36.7	44.6	0.6	12.3	0.1	95.8	0.6	104
6	Label 2	Water		7.3	1.6	35.9	43.0	0.6	12.1	0.1	93.1	1.8	102
7	Label 1	Sed		4.2	1.3	39.5	46.6	0.7	9.0	0.1	97.0	0.3	102
8	Label 2	Sed		4.9	1.4	36.7	46.8	0.6	9.2	0.1	94.7	1.6	101
9	Label 1	Water	90	6.2	1.7	30.8	44.6	0.6	13.9	0.1	91.5	1.0	99
10	Label 2	Water		5.6	1.6	33.4	45.6	0.7	13.5	0.1	94.8	2.0	102
11	Label 1	Sed		4.7	1.5	28.6	41.9	0.8	13.4	0.1	86.2	1.0	92
12	Label 2	Sed		4.8	1.4	31.8	46.9	0.7	13.6	0.1	94.4	2.5	102

Table 1. Mass Balance (% of applied radioactivity) including NER analysis

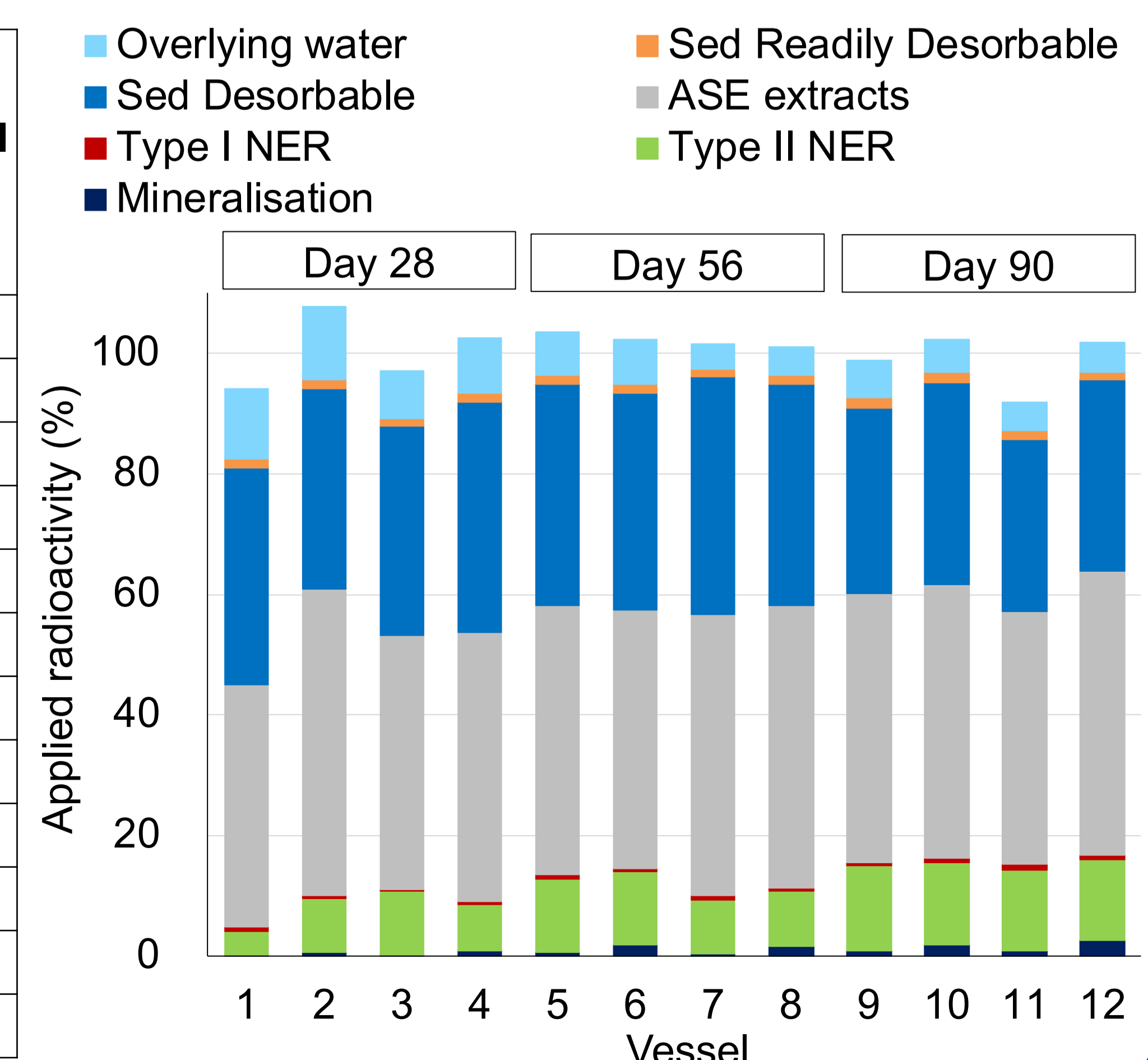


Figure 1. Mass balance of each vessel