Transformation of Organic Chemicals in Environmental Fate Metabolism Studies: A Comparison between Aquatic Sediment and Surface Water Test Systems (OECD 308 and 309)

Christiaan Wijntjes, Daniel Adam, Stefan Höger, Wolfgang Völkel
IES Ltd, Benkenstrasse 260, 4108 Witterswil, Switzerland

SETAC Europe 27th Annual Meeting
Brussels, Belgium, May 7th-11th, 2017
Poster n° TH236

Introduction

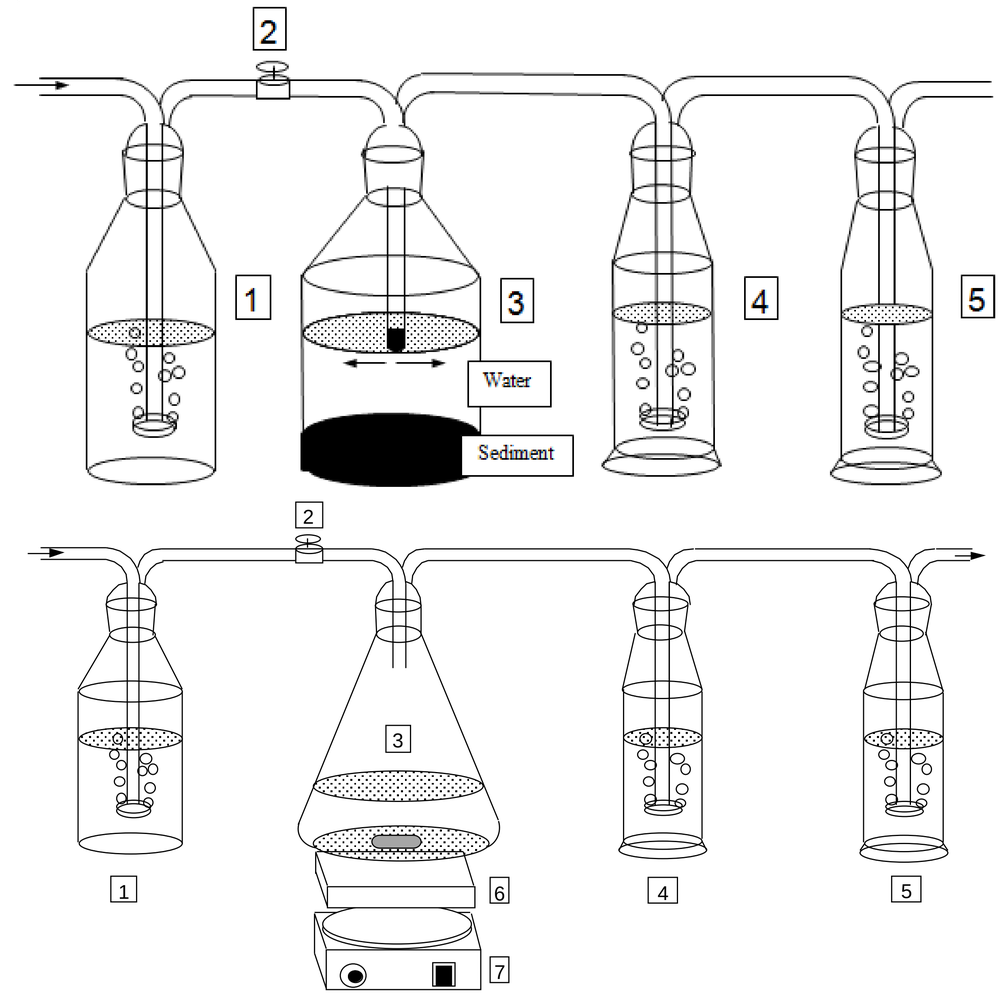
Higher-tier assessments include metabolism studies in aquatic sediment systems under aerobic and anaerobic incubation conditions (OECD 308) and aerobic degradation/ metabolism studies in natural surface water both with and without suspended sediment (OECD 309). Since the purpose of OECD 309 studies has recently been under discussion, the presented data intends to provide an insight into the influence of sediment on the transformation and/ or degradation velocity of organic chemicals in water/ sediment when compared to water only test systems.

Materials and Methods

OECD 308: Aerobic or anaerobic aquatic sediment test system
Studies performed at IES Ltd (2012-2017): 43 / Clients: 21
OECD 309: Surface water test system
Studies performed at IES Ltd (2012-2017): 46 / Clients: 18
No. of test items for which both (aerobic) study types have been conducted: 9

Study type / parameter	OECD 308	OECD 309
^{14}C-labelled test item(s)	All = 9 (with 1 to 2 labels)	
Water solubility	0.023-1449 mg/L	
Specific activity	1.8-11.9 MBq/mg	
Test concentrations	0.010-36.6 mg/L	Low dose: 0.01 mg/L High dose: 0.05-0.10 mg/L
Solvents	Water or organic solvents (OECD 309 including solvent control)	
Source of water and/or sediment	Lake, pond or river with ~pH 8 and 6-8 mg O_2/L	
Suspended solids (OECD 309)	-	One study with 1 g/L
Temperature/light	Incubation at 20-22°C in the dark	
Test duration	~100 days	60 (-90) days
Replicates	Duplicate samples at each interval	
Volume	~550-700 mL water and ~150-250 g wet sediment (sediment/water volume ratio between 1:3 and 1:4) in 1 L all-glass metabolism flasks	100-160 mL water in 300 mL Erlenmeyer flasks
Test system	Flow-through with NaOH and Ethylene glycol traps. Static system (OECD 308) or continuous agitation by magnetic stirrer (OECD 309)	
Degradation reference item (to assess microbial activity)	-	Benzoic acid
Microbial biomass (sediment)	Fumigation method [1]	-

Table 1: Data on aerobic OECD 308 & 309 studies performed at IES Ltd



(1) Water to moisten incoming air. (2) Valve to adjust the air flow. (3) Metabolism flask containing sediment and overlaying water (OECD 308) or Erlenmeyer flask containing natural water and eventually suspended sediment (gently stirred, OECD 309). (4) Ethylene glycol trap for org. volatiles. (5) 2N NaOH trap for $^{14}CO_2$. (6) Insulating foam. (7) Magnetic stirrer

Figure 1: Typical OECD 308 (top) and OECD 309 (bottom) test apparatus

Results

Test item	OECD 308				OECD 309			
	Major Metabolite(s)	DT_{50} Water/Total	CO_2	NER	Major Metabolite(s)	DT_{50} Water Low/High Dose	CO_2	Other Volatiles
1	M1 (<10%), M2 (<30%)	1-4h / 3-4d	≤35%	≤50%	M1 (≤12%), M3 (≤16%), M4 (≤18%), M5 (≤9%)	n.a. / 4-7d	≤60% (LD) ≤30% (HD)	<1%
2	none	85d / 95d	≤1%	≤8%	none	stable	<3%	<1%
3	up to 5, M1 (≤36% total)	0.6d / 0.6d (no parent in sed)	≤53%	≤35%	up to 6, M1 (≤28%)	n.a. / 2.5d	<57% (LD) <32% (HD)	<3%
4	M1 (≤44% wat; ≤20% sed)	90d / 100d	≤7%	<8%	M1 (≤16%)	3d (volatile parent)	<2%	<1%
5	M1 (≤77%), M2 (<98%)	0.2d / 0.7d	≤13%	<68%	M1 (≤100%), M2 (≤100%)	<1d	≤15%	<46%
6	M1 (≤11%, sed)	3-4d / 7-9d	≤26%	≤82%	none	31d / 120d	≤30% (LD) ≤50% (HD)	<1%
7	none	57-86h / stable	<4%	<6%	none	stable	<2%	<1%
8	M1 (≤19%, wat)	1d / 50d	≤45%	≤50%	M1 (≤20%)	41d / 24d	≤6%	<4%
9	none	19.5d / 28d	<7%	<36%	none	stable	<2%	<1%

Increasing water solubility

Values in % of applied radioactivity. NER: Non-extractable residues. LD: Low dose. HD: High dose. sed: Sediment. wat: Water. n.a.: Not available

Table 2: Degradation results for each of the nine test items in the OECD 308 and 309 test systems

Summary

- The half-life (DT_{50}) of tested compounds tends to be higher in OECD 309 than in OECD 308 studies, where sediment present.
- For three out of nine test compounds, the formation and/or relative amount of metabolites significantly differed between both study types.
- No correlation between water solubility and study outcome was observed.
- For one compound with low water solubility, suspended soil particles (1 g/L; OECD 309) tend to slightly shorten test item dissipation rates for the water phase (data overview not shown on present poster). Formation of different metabolites was correlated to the test system: Differences were observed between pond and river, as well as for the presence of suspended soil.

However, for all points mentioned above, exceptions have been observed.

Conclusion

- The absence of sediment (pelagic test) may lead to diverse degradation behavior.
- In general, OECD 308 studies may be more appropriate for simulating stagnant systems (e.g. ponds), while OECD 309 studies may better reflect disturbed i.e. flowing systems (e.g. rivers).
- Considering the relative simplicity in conducting OECD 309 studies, this study type may offer a convenient behavior assessment, especially for more delicate compounds, prior to conducting more sophisticated OECD 308 studies.

References

[1] Vance E.D., Brookes P.C. and Jenkinson D.S., 1987. An extraction method for measuring soil microbial C. Soil Biol. Biochem. 19, 703-708.