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Environmental risk evaluation report: Annex C: Consideration of hydrolysis

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Steve Killeen

Head of Science

Introduction

Although all of the aryl phosphate esters considered in this series are likely to be susceptible to hydrolysis, the available information indicates (with the exception of tetraphenyl resorcinol diphosphate) that the rate of hydrolysis in surface water is likely to be very slow at near neutral pHs, and so a hydrolysis rate was not included in the calculation of predicted environmental concentrations (PECs) given in most of the main risk evaluation reports (a hydrolysis half-life in surface water of 21 days was included in the assessment of tetraphenyl resorcinol diphosphate). However, in some situations (such as low or high pH environments) the hydrolysis rates of all the aryl phosphate esters considered could become important and so this annex considers the effect of inclusion of a hydrolysis rate on the overall conclusions of the assessment.

As well as surface water, hydrolysis could also become an important degradation process in soil and sediment. Degradation rate constants used in the main risk assessment report were extrapolated mainly from results from standard ready or inherent biodegradation tests using the methods outlined in the Technical Guidance Document (TGD). There is considerable uncertainty in the degradation rate constants obtained by this method. At present, it is not possible to take hydrolysis into account in degradation rates for soil and sediment using the methods outlined in the TGD and so the approach used here investigated the sensitivity of the conclusions of the risk assessment to the overall degradation rate in soil and sediment.

For each substance, EUSES 2.0 was run several times. The benchmark case used the degradation rates for surface water, sediment and soil outlined in the main risk evaluation reports. Further scenarios were considered using different combinations of hydrolysis rates and sediment and soil degradation rates. In each case, a standard scenario was used (local releases of 0.1 kg/day to air and 0.1 kg/day to waste water; regional and continental releases of 0.1 kg/day to each of air, waste water, surface water and industrial soil). The results of this analysis are summarised in Table C 1.

The following points are evident from Table C 1.

- Inclusion of a hydrolysis rate for surface water has no effect on predicted local concentrations for any of the substances. A small effect on predicted regional concentrations for surface water and sediment is seen for most substances. The effect is generally largest for substances considered to be inherently biodegradable in the assessment, but the reduction is only around a factor of two using a relatively rapid hydrolysis half-life of 20 days. Therefore it can be concluded that the assessments are relatively insensitive to the inclusion of a hydrolysis rate.
- PECs for sediment and soil for tricresyl phosphate and cresyl diphenyl phosphate are relatively insensitive to the soil and sediment degradation rate used (generally PECs were within a factor of two of the benchmark case over the range of degradation rates considered).
- Local and regional PECs for sediment and soil for triphenyl phosphate, trixylenyl phosphate, isopropylphenyl diphenyl phosphate, tris(isopropylphenyl) phosphate, tertbutyl phenyl diphenyl phosphate, tetraphenyl resorcinol diphosphate, 2-ethylhexyl diphenyl phosphate and isodecyl diphenyl phosphate are more sensitive to the degradation rate used for sediment and soil, with the effect being largest for substances considered to be inherently biodegradable in the assessment. It may thus be possible to refine sediment and soil PECs significantly for these substances by carrying out further testing[1] to investigate the actual degradation (mineralization) half-life in sediment and soil under relevant environmental conditions.

[1] The half-life determined in such a test would be the result of degradation by both biodegradation and hydrolysis to biodegradable substances.

Table C 1 Sensitivity of PECs to hydrolysis half-life

Substance	Endpoint	Predicted concentration[a]					
		Base case	Hydrolysis half-life		Soil and sediment degradation half-life		
			20 days	50 days	50 days	100 days	150 days
Triphenyl phosphate	PEC_{local} surface water	4.1×10^{-4}	4.1×10^{-4}	4.1×10^{-4}	4.1×10^{-4}	4.1×10^{-4}	4.1×10^{-4}
	PEC_{local} sediment	0.089	0.089	0.089	0.089	0.089	0.089
	PEC_{local} agricultural soil	0.13	0.13	0.13	0.063	0.075	0.087
	$PEC_{regional}$ surface water	3.6×10^{-7}	2.5×10^{-7}	3.1×10^{-7}	3.4×10^{-7}	3.4×10^{-7}	3.5×10^{-7}
	$PEC_{regional}$ sediment	8.1×10^{-5}	5.7×10^{-5}	6.9×10^{-5}	2.3×10^{-5}	4.1×10^{-5}	5.4×10^{-5}
	$PEC_{regional}$ agricultural soil	2.2×10^{-6}	2.2×10^{-6}	2.2×10^{-6}	3.8×10^{-7}	7.5×10^{-7}	1.1×10^{-6}
Tricresyl phosphate	PEC_{local} surface water	4.8×10^{-4}	4.8×10^{-4}	4.8×10^{-4}	4.8×10^{-4}	4.8×10^{-4}	4.8×10^{-4}
	PEC_{local} sediment	0.050	0.050	0.050	0.050	0.050	0.050
	PEC_{local} agricultural soil	0.037	0.037	0.037	0.042	0.050	0.059
	$PEC_{regional}$ surface water	4.1×10^{-7}	2.8×10^{-7}	3.5×10^{-7}	4.0×10^{-7}	4.1×10^{-7}	4.1×10^{-7}
	$PEC_{regional}$ sediment	4.4×10^{-5}	3.0×10^{-5}	3.7×10^{-5}	1.4×10^{-5}	2.3×10^{-5}	3.1×10^{-5}
	$PEC_{regional}$ agricultural soil	2.0×10^{-7}	2.0×10^{-7}	2.0×10^{-7}	3.3×10^{-7}	6.7×10^{-7}	1.0×10^{-6}
Trixylenyl phosphate	PEC_{local} surface water	2.5×10^{-3}	2.5×10^{-3}	2.5×10^{-3}	2.5×10^{-3}	2.5×10^{-3}	2.5×10^{-3}
	PEC_{local} sediment	0.46	0.46	0.46	0.46	0.46	0.46
	PEC_{local} agricultural soil	0.64	0.64	0.64	0.076	0.090	0.10
	$PEC_{regional}$ surface water	1.9×10^{-6}	7.6×10^{-7}	1.2×10^{-6}	1.3×10^{-6}	1.3×10^{-6}	1.4×10^{-6}
	$PEC_{regional}$ sediment	6.0×10^{-4}	2.4×10^{-4}	3.8×10^{-4}	7.6×10^{-5}	1.4×10^{-4}	1.8×10^{-4}
	$PEC_{regional}$ agricultural soil	2.8×10^{-5}	2.8×10^{-5}	2.8×10^{-5}	5.1×10^{-7}	1.1×10^{-6}	1.5×10^{-6}

Table C 1 continued.

Substance	Endpoint	Predicted concentration[a]					
		Base case	Hydrolysis half-life		Soil and sediment degradation half-life		
			20 days	50 days	50 days	100 days	150 days
Cresyl diphenyl phosphate	PEC_{local} surface water	1.4×10^{-3}	1.4×10^{-3}	1.4×10^{-3}	1.4×10^{-3}	1.4×10^{-3}	1.4×10^{-3}
	PEC_{local} sediment	0.071	0.071	0.071	0.071	0.071	0.071
	PEC_{local} agricultural soil	0.033	0.033	0.033	0.029	0.034	0.040
	$PEC_{regional}$ surface water	9.1×10^{-7}	4.8×10^{-7}	6.7×10^{-7}	8.9×10^{-7}	9.1×10^{-7}	9.2×10^{-7}
	$PEC_{regional}$ sediment	2.6×10^{-5}	1.4×10^{-5}	1.9×10^{-5}	1.7×10^{-5}	2.8×10^{-5}	3.6×10^{-5}
	$PEC_{regional}$ agricultural soil	5.2×10^{-7}	5.2×10^{-7}	5.2×10^{-7}	2.9×10^{-7}	5.8×10^{-7}	8.7×10^{-7}
Isopropyl phenyl diphenyl phosphate	PEC_{local} surface water	1.1×10^{-3}	1.1×10^{-3}	1.1×10^{-3}	1.1×10^{-3}	1.1×10^{-3}	1.1×10^{-3}
	PEC_{local} sediment	0.14	0.14	0.14	0.14	0.14	0.14
	PEC_{local} agricultural soil	0.24	0.24	0.24	0.052	0.062	0.072
	$PEC_{regional}$ surface water	9.2×10^{-7}	4.9×10^{-7}	6.8×10^{-7}	7.8×10^{-7}	8.0×10^{-7}	8.2×10^{-7}
	$PEC_{regional}$ sediment	1.7×10^{-4}	9.0×10^{-5}	1.3×10^{-4}	3.2×10^{-5}	5.6×10^{-5}	7.5×10^{-5}
	$PEC_{regional}$ agricultural soil	7.3×10^{-6}	7.3×10^{-6}	7.3×10^{-6}	4.2×10^{-7}	8.3×10^{-7}	1.3×10^{-6}
Tris(isopropyl phenyl) phosphate	PEC_{local} surface water	1.4×10^{-3}	1.4×10^{-3}	1.4×10^{-3}	1.4×10^{-3}	1.4×10^{-3}	1.4×10^{-3}
	PEC_{local} sediment	0.42	0.42	0.42	0.42	0.42	0.42
	PEC_{local} agricultural soil	0.73	0.73	0.73	0.086	0.10	0.12
	$PEC_{regional}$ surface water	1.2×10^{-6}	5.7×10^{-7}	8.4×10^{-7}	8.0×10^{-7}	8.4×10^{-7}	8.7×10^{-7}
	$PEC_{regional}$ sediment	6.8×10^{-4}	3.2×10^{-4}	4.6×10^{-4}	7.9×10^{-5}	1.4×10^{-4}	1.9×10^{-4}
	$PEC_{regional}$ agricultural soil	3.3×10^{-5}	3.3×10^{-5}	3.3×10^{-5}	5.7×10^{-7}	1.1×10^{-6}	1.7×10^{-6}

Table C 1 continued.

Substance	Endpoint	Predicted concentration[a]					
		Base case	Hydrolysis half-life		Soil and sediment degradation half-life		
			20 days	50 days	50 days	100 days	150 days
tert-Butyl phenyl diphenyl phosphate	PEC_{local} surface water	2.0×10^{-3}	2.0×10^{-3}	2.0×10^{-3}	2.0×10^{-3}	2.0×10^{-3}	2.0×10^{-3}
	PEC_{local} sediment	0.21	0.21	0.21	0.21	0.21	0.21
	PEC_{local} agricultural soil	0.10	0.10	0.10	0.050	0.060	0.069
	$PEC_{regional}$ surface water	1.3×10^{-6}	6.0×10^{-7}	8.8×10^{-7}	1.2×10^{-6}	1.2×10^{-6}	1.2×10^{-6}
	$PEC_{regional}$ sediment	1.4×10^{-4}	6.5×10^{-5}	9.5×10^{-5}	4.0×10^{-5}	7.0×10^{-5}	9.3×10^{-5}
	$PEC_{regional}$ agricultural soil	2.3×10^{-6}	2.3×10^{-6}	2.3×10^{-6}	3.9×10^{-7}	7.9×10^{-7}	1.2×10^{-6}
Tetraphenyl resorcinol diphosphate	PEC_{local} surface water	2.7×10^{-3}	2.7×10^{-3}	2.7×10^{-3}	2.7×10^{-3}	2.7×10^{-3}	2.7×10^{-3}
	PEC_{local} sediment	0.43	0.43	0.43	0.43	0.43	0.43
	PEC_{local} agricultural soil	0.60	0.60	0.60	0.071	0.084	0.099
	$PEC_{regional}$ surface water	7.5×10^{-7}	7.3×10^{-7}	1.1×10^{-6}	6.1×10^{-7}	6.3×10^{-7}	6.3×10^{-7}
	$PEC_{regional}$ sediment	2.1×10^{-4}	2.0×10^{-4}	3.0×10^{-4}	3.2×10^{-5}	5.5×10^{-5}	7.3×10^{-5}
	$PEC_{regional}$ agricultural soil	2.7×10^{-5}	2.7×10^{-5}	2.7×10^{-5}	5.0×10^{-7}	1.0×10^{-6}	1.5×10^{-6}
2-Ethylhexyl diphenyl phosphate	PEC_{local} surface water	9.7×10^{-4}	9.7×10^{-4}	9.7×10^{-4}	9.7×10^{-4}	9.7×10^{-4}	9.7×10^{-4}
	PEC_{local} sediment	0.20	0.20	0.20	0.20	0.20	0.20
	PEC_{local} agricultural soil	0.10	0.10	0.10	0.067	0.079	0.093
	$PEC_{regional}$ surface water	7.3×10^{-7}	4.1×10^{-7}	5.6×10^{-7}	6.6×10^{-7}	6.8×10^{-7}	7.0×10^{-7}
	$PEC_{regional}$ sediment	1.6×10^{-4}	8.9×10^{-5}	1.2×10^{-4}	4.4×10^{-5}	7.7×10^{-5}	1.0×10^{-4}
	$PEC_{regional}$ agricultural soil	2.5×10^{-6}	2.5×10^{-6}	2.5×10^{-6}	4.2×10^{-7}	8.5×10^{-7}	1.3×10^{-6}

Table C 1 continued.

Substance	Endpoint	Predicted concentration[a]					
		Base case	Hydrolysis half-life		Soil and sediment degradation half-life		
			20 days	50 days	50 days	100 days	150 days
Isodecyl diphenyl phosphate	PEC_{local} surface water	1.8×10^{-3}	1.8×10^{-3}	1.8×10^{-3}	1.8×10^{-3}	1.8×10^{-3}	1.8×10^{-3}
	PEC_{local} sediment	0.27	0.27	0.27	0.27	0.27	0.27
	PEC_{local} agricultural soil	0.52	0.52	0.52	0.062	0.074	0.086
	$PEC_{regional}$ surface water	1.4×10^{-6}	6.5×10^{-7}	9.7×10^{-7}	1.1×10^{-6}	1.1×10^{-6}	1.1×10^{-6}
	$PEC_{regional}$ sediment	3.7×10^{-4}	1.7×10^{-4}	2.5×10^{-4}	5.1×10^{-5}	8.9×10^{-5}	1.2×10^{-4}
	$PEC_{regional}$ agricultural soil	2.3×10^{-5}	2.3×10^{-5}	2.3×10^{-5}	4.2×10^{-7}	8.4×10^{-7}	1.3×10^{-6}

Notes: a) The concentrations have the following units throughout:
surface water mg/l
sediment mg/kg wet weight
agricultural soil mg/kg wet weight

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