Examining the relevance of the microplastic-associated additive fraction in environmental compartments

SUPPORTING INFORMATION

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Table S1. Examples of relevant additives for the modelling undertaken in the present study, together with their CAS number, $\log K_{ow}$ or logP, their function and application, typical concentrations in plastic products and examples of concentrations reported for matrices such as sediment and sewage sludge or effluents.

Figure S1. Simulated variation in the proportion of model plastic-incorporated chemical additive (CAD) in a sample ($N_{P\text{-}CAD}/N_{S\text{-}CAD}$) as a function of the organic carbon (OC) content to plastic x ratio of

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the sample and the K_{pw} and K_{oc} of the chemical additive. For this simulation, the $C_{CAD\text{-}free}$ was set to 1 ng L^{-1}, f_{Px} to 0.2, P_{Px} to 0.001 and the proportion of CAD in the plastic x = 5 %.

Figure S2. Simulated distribution of a model chemical additive (CAD) between presence as a plastic additive, sorbed to plastic, and sorbed to organic carbon (OC) as a function of the OC content to plastic x ratio of the sample and the proportion of additive-loaded plastic f_{Px}. For this simulation, the $C_{CAD\text{-}free}$ was set to 1 ng L^{-1}, $\log K_{pw}K_{oc}$ = 5, P_{Px} = 0.001, P = 0.08, and the proportion of CAD in the plastic x = 5 %.

Figure S3. Simulated concentration ratios of a model chemical additive (CAD) over that of a reference chemical for (i) freely dissolved concentrations (C_{Free}) and concentrations for sorbed to particulate (C_{Part}) organic carbon (OC) and plastic with and without the presence of the CAD as an additive in a proportion f_{Px} of additive-loaded plastic. For this simulation, the $C_{CAD\text{-}free}$ was set to 0.03 ng L^{-1}, $\log K_{pw}$ and K_{oc} = 6, P = 0.01, and the proportion of CAD in the plastic x = 5 %. The C_{Free} was set to 0.1 ng L^{-1} for the reference chemical, and $\log K_{pw}$ and K_{oc} = 5.

Figure S4. Simulation of the proportion of a model chemical additive dissipating from microplastic particles with a diameter of 1, 0.1, 0.01, 0.001, 0.0001, and 0.0001 mm over periods of 0.5 and 10 days, 1 and 10 years. These simulations assume that transport in the polymer is the main resistance to mass transfer of the chemical from the particle to the outer environment.

Table S2. Examples of reported diffusion coefficients of additives in plastics or plastic particles.

Examples of relevant additives

Table S1 presents a range of example additives relevant to the modelling undertaken in this study. This list is not exhaustive but mostly includes substances identified through ECHA's plastic additive mapping exercise. A few of these substances have high pKa but are not expected to be dissociated at pH of 6-8. Substances included are mostly flame retardants, plasticisers and UV stabilisers. More comprehensive lists of relevant chemicals can be found elsewhere[1-6].

Table S1. Examples of relevant additives for the modelling undertaken in the present study, together with their CAS number, $logK_{ow}$ or logP, their function and application, typical concentrations in plastic products and examples of concentrations reported for matrices such as sediment and sewage sludge or effluents.

	Additive	CAS number	$logK_{ow}$ or logP	Function	Application (plastic)	Typical concentration (%)	Typical concentrations ranges in sediment (ng g^{-1} dw)	Typical concentrations in sewage sludge (ng g^{-1} dw) and/or effluent (ng L^{-1})	References
1	1,1'-(ethane-1,2-diyl)bis(pentabromobenzene)	84852-53-9	11.1	Flame retardant	PUR; PVC	15-35			
2	Short chain chlorinated paraffins (SCCPs)			Flame retardant/plasticiser			320-6600	<57-1421 ng g^{-1} 16-416 ng L^{-1}	7, 8,9
3	Medium chain chlorinated paraffins (MCCPs)	85535-85-9	5.5-8.4	Flame retardant/plasticiser	PUR; PVC	15	18-38000	30-9700 ng g^{-1} 455±177 ng L^{-1}	7, 10, 11 8, 9, 12
4	Dechlorane plus	13560-89-9	8	Flame retardant	polyolefin	3	0.06-586	0.9-75.1 ng g^{-1}	13-15
5	Bis(2-Ethylhexyl) Phthalate	117-81-7	7.5	Plasticiser	PUR; PVC; ABS; PS	2-35	9-16000	27900-180000 ng g^{-1} 1740-182000 ng L^{-1}	16-21
6	Dibutyl phthalate	84-74-2	4.7	Plasticiser	PUR; PVC	10-35	60-2080	200-1700 ng g^{-1} 200-10400 ng L^{-1}	18
7	Diisononylphthalate	28553-12-0;68515-48-0	9.6	Plasticiser	PUR; PVC	10-35			
8	Triphenyl phosphate	115-86-6	4.6	Plasticiser/flame retardant			0.42-316.5	4.4-66.8 ng g^{-1} <2.6-170 ng L^{-1}	22-26
9	Octabenzone	1843-05-6	6.8	UV stabiliser	Polyolefin; PUR; ABS; PVC; PMMA; PC; PS	0.2-5			
10	Bumetrizole (UV-326)	3896-11-5	5.6	UV stabiliser	Polyolefin; PUR; ABS; PVC; PMMA; PC; PS	0.3-1	3-28	4-3390 ng g^{-1} 3.6±0.7 ng L^{-1}	27-29
11	2-(2′-Hydroxy-3′,5′-di-tert-butylphenyl)-5-chlorobenzotriazole (UV-327)	3864-99-1		UV stabiliser			0.4-16	1.53-160 ng g^{-1} <0.5-31 ng L^{-1}	27-29

12	Irganox 245	36443-68-2	6.9	Antioxidant	Polyolefin; PUR; ABS; PVC; PMA; PC; PS	0.005-3			
13	Dibutyl adipate	105-99-7	3.1	Plasticiser	PUR; PVC	10-35			
14	Phenol, 2-(2H-benzotriazol-2-yl)-4,6-bis(1,1-dimethylpropyl)- (UV328)	25973-55-1	7.4	UV stabiliser	Polyolefin	0.1-1	2-240	3.5 -5920 ng g^{-1} 2.6-21 ng L^{-1}	27-29
15	2-(2′-hydroxy-5′-(1,1,3,3-tetramethylbutyl)phenyl)benzotriazole (UV329)	3147-75-9		UV stabiliser			1.8-47	0.57-3303 ng g^{-1} <5.6-8.5 ng L^{-1}	27-29
16	Decabromodiphenyl ethane (DBDPE)	84852-53-9	11.1	Flame retardant	Thermoplastics, PP, polyester and epoxy		24	6.43-1440 ng g^{-1}	30, 31
17	Decabromodiphenyl ether (BDE-209)	1163-19-5	10.4	Flame retardant	HIPS; polyolefin		1280	1420-14200 ng g^{-1}	30, 31

$\log K_{ow}$ or logP are from pubchem (https://pubchem.ncbi.nlm.nih.gov/); Application and typical concentrations are from the European Chemical agency's plastic additive mapping exercise (ECHA https://echa.europa.eu/mapping-exercise-plastic-additives-initiative) for chemicals 1-12;
PUR: Polyurethane; PVC: polyvinylchloride; PC: polycarbonate; PS: polystyrene; ABS: acrylonitrile butadiene styrene; PMMA: polymethylmethacrylate, HIPS: High impact polystyrene

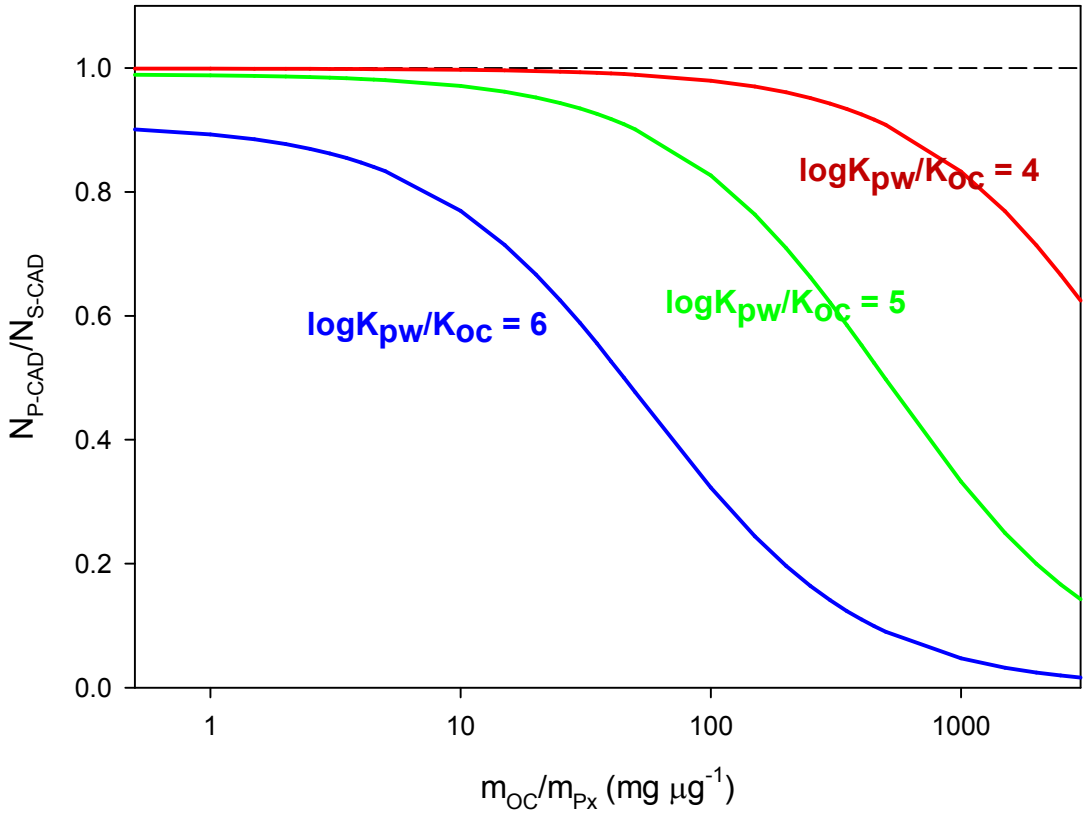
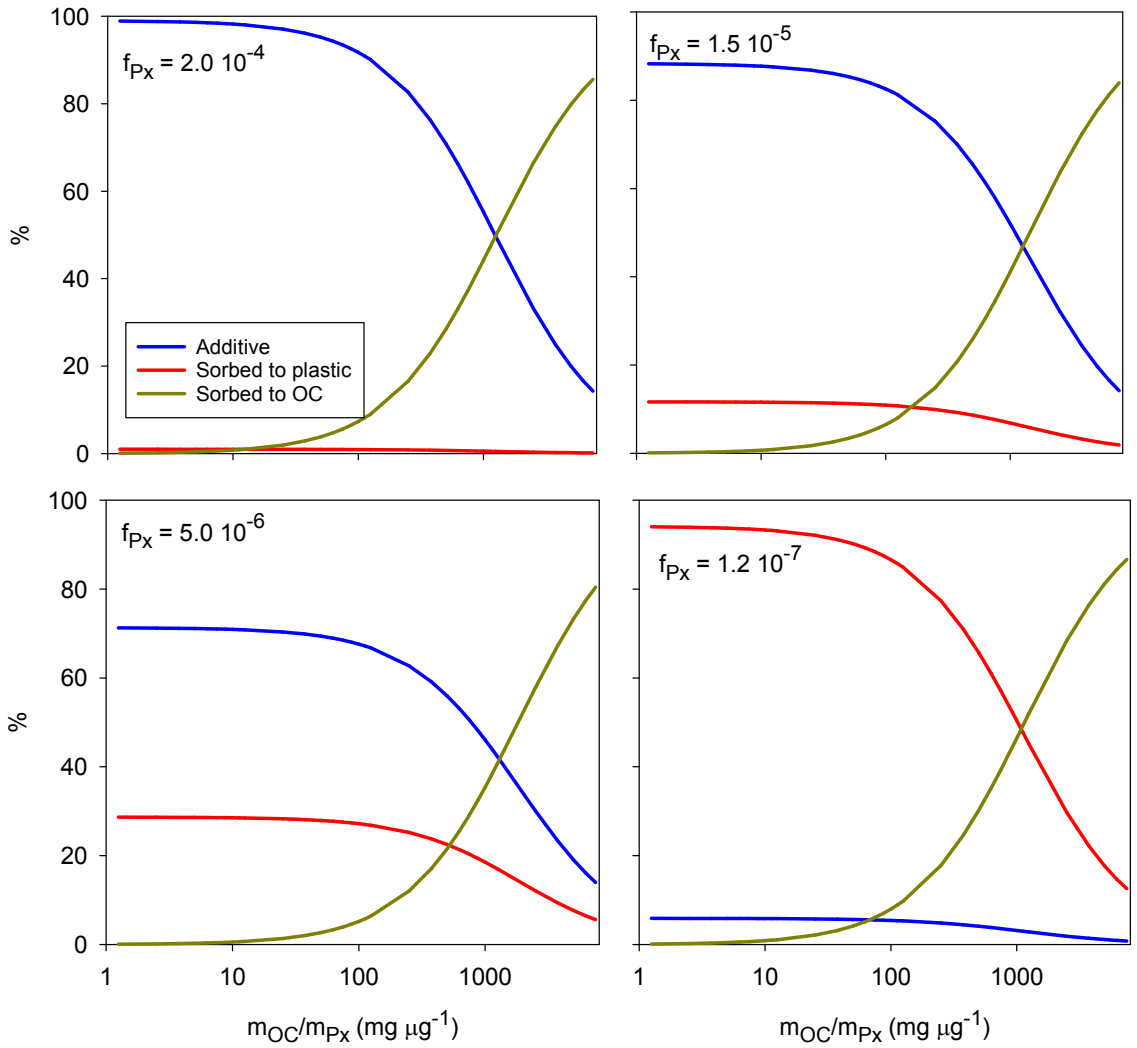


Figure S1. Simulated variation in the proportion of model plastic-incorporated chemical additive (CAD) in a sample ($N_{P\text{-}CAD}/N_{S\text{-}CAD}$) as a function of the organic carbon (OC) content to plastic x ratio of the sample and the K_{pw} and K_{oc} of the chemical additive. For this simulation, the $C_{CAD\text{-}free}$ was set to 1 ng L^{-1}, f_{Px} to 0.2, P_{Px} to 0.001 and the proportion of CAD in the plastic x = 5%.



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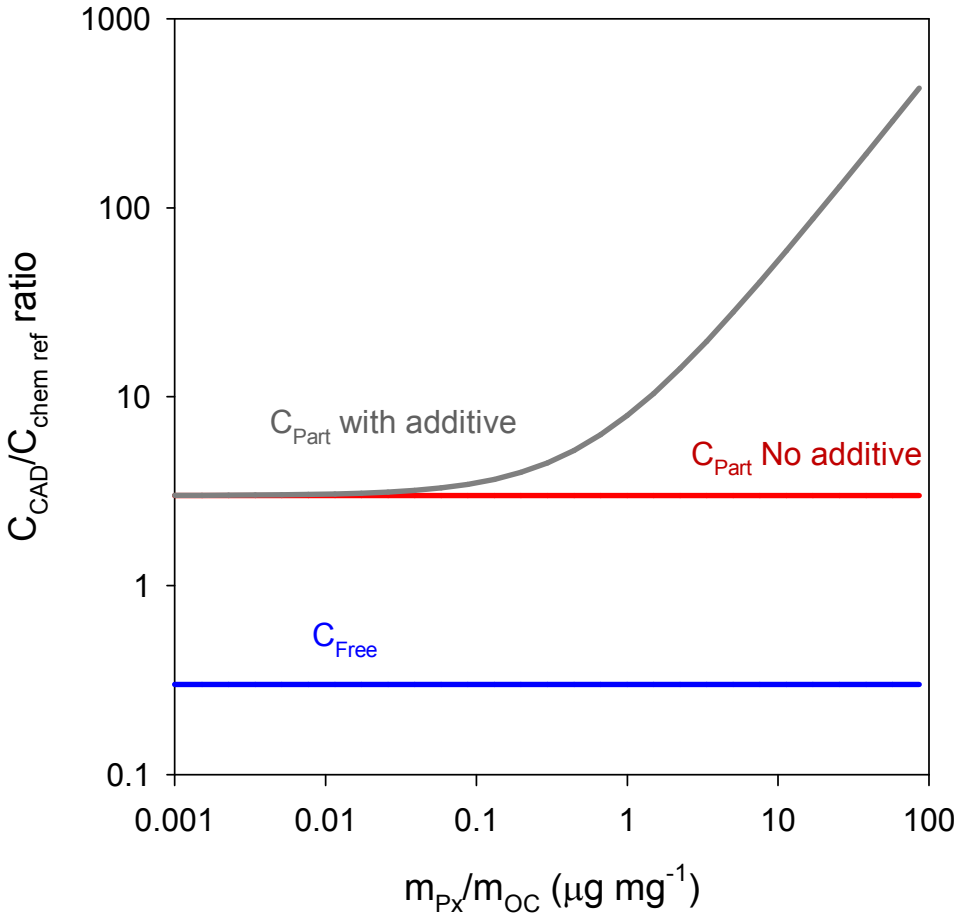

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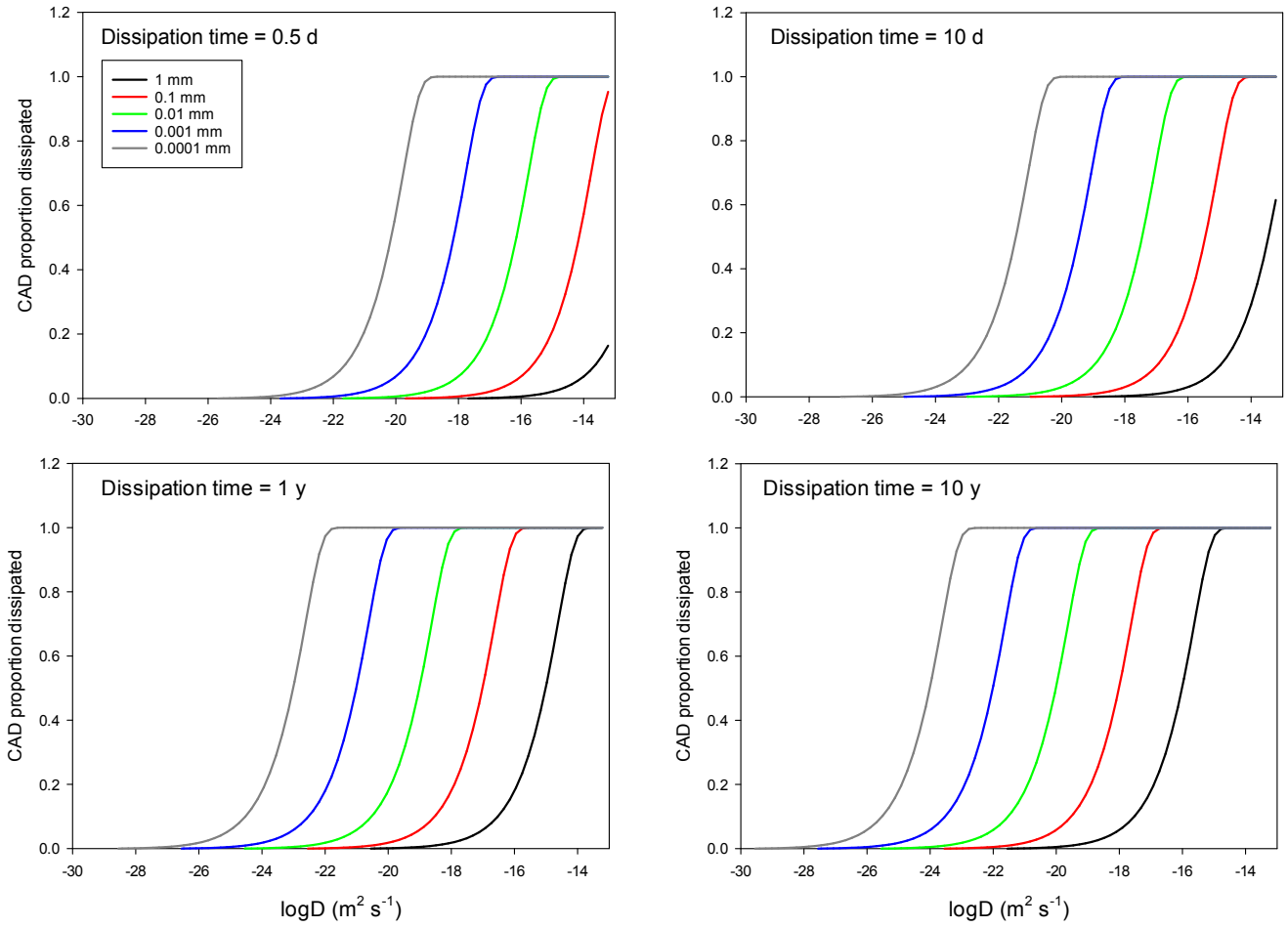

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Table S2. Examples of reported diffusion coefficients of additives in plastics or plastic particles.

Additive	Plastic/polymer	Diffusion coefficient (m^2 s^{-1}), logD	Temperature (°C)	Reference
Irganox 1010	Poly(propylene-co-ethylene) copolymer	-13.9 to -16.2	40	32
Irganox 1076	Polypropylene	-15.2	40	33
Irgafos 168	Polypropylene	-16.4 to -17	40	33
DEHP	Polypropylene	-14.4	40	33
Tinuvin P	Polypropylene	-13.8	40	33
Triphenyl phosphate	Low density polyethylene	< -15	20	34
PBDEs	Acrylonitrile butadiene styrene	-21.9 to -25.5	10	35
PBDEs	Low density polyethylene	-13.2 to < -20.8	20	36
BTBPE	Acrylonitrile butadiene styrene	-24 and -25.5	10	37
PBDEs	Polystyrene	-16.4 to -18.1	25	38
PBDEs	Acrylonitrile butadiene styrene	-18.8 to -19.7	25	38
PBDEs	Polypropylene	-15.9 to -17.1	25	38

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