Electronic Supplementary Material (ESI) for Environmental Science: Processes & Impacts.

Supplementary information

Evaluation of the OECD P_{OV} and LRTP Screening Tool for Estimating the Long-range Transport of Organophosphate Esters

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Table S1: Acronym, IUPAC name, CAS number and molecular weight (MW) [g mol^{-1}] of the tested OPEs.

Acronym	Name	CAS number	MW [g mol^{-1}]
BCMP-BCEP	Tetrakis(2-chloroethyl)dichloroisopentyldiphosphate	38051-10-4	583
BDCPP	Bis(1,3-dichloro-2-propyl) phosphate	72236-72-7	320
BEHP	Bis(2-ethylhexyl) phosphate	298-07-7	322
BMPPP	Bis(methylphenyl) phenyl phosphate	26446-73-1	354
BPA-BDPP	Bisphenol A bis(diphenyl phosphate)	5945-33-5, 181028-79-5	693
BPDP	Di-tert-butylphenyl diphenyl phosphate	56803-37-3	382
DCP	Diphenyl cresyl phosphate	26444-49-5	340
DOPO	9,10-Dihydro-9-oxa-10-phosphaphenanthrene-10-oxide	35948-25-5	216
EHDPP	Ethylhexyldiphenyl phosphate	1241-94-7	362
IDDPP	Isodecyl diphenyl phosphate	29761-21-5	390
MC 984	Tris(2,3-dichloro-1-propyl)phosphate	66108-37-0	582
PBDMPP	Tetrakis(2,6-dimethylphenyl)-m-phenylene biphosphate	139189-30-3	687
PBDPP	Resorcinol bis(diphenyl phosphate)	57583-54-7, 125997-21-9	574
IPPP	Isopropylphenyl phosphate	68937-41-7	453
TBOEP	Tris(2-butoxyethyl) phosphate	78-51-3	398
TCEP	Ethanol, 2-chloro-, phosphate (3:1)	115-96-8	285
TCIPP	Tris(1-chloro-2-propyl)phosphate	13674-84-5	328
TCP	Tris(cresyl) phosphate	1330-78-5	368
TDBPP	1-Propanol, 2,3-dibromo-, 1,1',1''-phosphate	126-72-7	698
TDCIPP	Tris(1,3-dichloroisopropyl)phosphate	13674-87-8	431
TDMPP	Tris(3,5-dimethyl phenyl) phosphate	9006-37-5	410
TEHP	Tris(2-ethylhexyl) phosphate	78-42-2	435
TEP	Triethyl phosphate	78-40-0	182
TIBP	Triisobutyl phosphate	126-71-6	266
TiPP	Triisopropyl phosphate	513-02-0	224
ToCP	Tri(o-cresyl) phosphate	78-30-8	368
TMP	Trimethyl phosphate	512-56-1	140
TnBP	Tri *n* butyl phosphate	126-73-8	266
TmCP	Tri(m-cresyl) phosphate	563-04-2	368
TpCP	Tri(p-cresyl) phosphate	78-32-0	368
TPhP	Triphenyl phosphate	115-86-6	326
T2iPPP	Tris(2-isopropyl phenyl) phosphate	64532-95-2	453
TTBNPP	1-Propanol, 3-bromo-2,2-bis(bromomethyl)-, 1,1',1''-phosphate	19186-97-1	1018
TTBPP	Tris(4-tert-butylphenyl) phosphate	78-33-1	495
TXP	Trixylyl phosphate	25155-23-1	410

Table S2: Input data for the Tool predictions including molecular weight (MW) [g mol^{-1}], the partitioning coefficients between air and water and octanol and water (log K_{AW} and log K_{OW}, respectively) and the environmental half-lives ($t_{1/2}$) in air, water and soil [h].

Chemical	**MW [g mol^{-1}]**	**log K_{AW}**	**log K_{OW}**	**$t_{1/2}$ Air**	**$t_{1/2}$ Water**	**$t_{1/2}$ Soil**
BCMP-BCEP	583	-12.20	3.07	3	4320	87600
BDCPP	320	-8.82	2.05	21	8760	6384
BEHP	322	-5.77	5.91	4	6660	6144
BMPPP	354	-5.70	5.80	10	912	3780
BPA-BDPP	693	-5.41	7.15	11	1440	2880
BPDP	382	-5.38	6.61	8	912	3684
DCP	340	-5.75	4.54	22	900	1800
DOPO	216	-5.65	2.68	43	900	1800
EHDPP	362	-4.99	5.80	8	780	54168
IDDPP	390	-4.75	6.11	7	2256	72000
IPPP	453	-4.92	9.07	4	1440	547
MC 984	582	-8.10	5.66	7	4320	47340
PBDMPP	687	-10.58	11.04	5	4320	8640
PBDPP	574	-8.23	6.29	12	912	1800
TBOEP	398	-8.93	3.75	2	456.4	2664
TCEP	285	-6.04	1.63	12	2172	4008
TCIPP	328	-6.16	2.68	7	3270	47520
TCP	368	-5.66	5.93	19	909	720
TDBPP	698	-9.78	4.29	9	1440	2880
TDCIPP	431	-6.97	3.89	12	4320	51912
TDMPP	410	-5.53	7.49	3	912	4320
TEHP	435	-3.39	9.42	3	240.4	4320
TEP	182	-4.87	0.88	3	360	720
TIBP	266	-3.34	3.65	3	360	720
TiPP	224	-4.25	2.12	3	360	720
ToCP	368	-5.66	5.95	19	909	5256
TMP	140	-4.99	-0.65	33	360	4320
TnBP	266	-3.88	4.00	3	208.2	8112
TmCP	368	-5.66	5.95	9	909	52224
TpCP	368	-5.66	5.95	19	909	13080
TPhP	326	-4.49	4.62	24	795	768
T2iPPP	453	-4.92	8.53	13	912	4320
TTBNPP	1018	-11.10	8.05	3	4320	8640
TTBPP	495	-4.55	9.94	18	4320	6120
TXP	410	-5.53	7.98	3	1440	547

Table S3: Sensitivity [%] of the predicted persistence (P_{OV}) of OPEs to a change by a factor of 1.1 of individual input parameters; Sensitivities of > 1% are marked green.

	Sensitivity to individual input parameters				
Chemical	Log K_{AW}	Log K_{OW}	$t_{1/2}$ air	$t_{1/2}$ water	$t_{1/2}$ soil
BCMP-BCEP	5E-09	1E-02	2E-16	0.8	13
BDCPP	1E-07	1E-09	7E-10	17	5E-06
BEHP	1E-03	1E-04	6E-06	15	1.4
BMPPP	8E-06	1E-04	9E-08	3E-03	17
BPA-BDPP	8E-07	7E-05	4E-08	7E-03	17
BPDP	3E-06	7E-05	5E-08	3E-03	17
DCP	1E-04	9E-04	4E-06	2E-02	17
DOPO	5E-03	1E-02	7E-04	1.0	15
EHDPP	2E-04	9E-05	6E-12	2E-07	7E-04
IDDPP	2E-05	2E-04	7E-08	2E-03	17
MC 984	7E-08	2E-04	4E-11	8E-03	17
PBDMPP	6E-16	1E-07	0.0	1E-02	17
PBDPP	5E-09	5E-05	3E-12	5E-03	17
IPPP	2E-05	9E-05	6E-07	11	7E-04
TBOEP	1E-06	6E-03	1E-10	2E-02	17
TCEP	9E-03	3E-03	2E-04	9.2	5.8
TCIPP	2E-03	2E-02	2E-05	1.8	12
TCP	1E-03	2E-04	7E-05	17	9E-04
TDBPP	1E-07	4E-03	3E-12	0.15	52
TDCIPP	5E-05	4E-03	3E-07	8E-02	16
TDMPP	2E-07	8E-05	3E-09	3E-03	17
TEHP	1E-07	5E-06	2E-09	4E-04	17
TEP	6E-02	2E-03	2E-04	4.4	11
TIBP	4E-03	1E-02	1E-05	4E-02	17
TiPP	2E-02	3E-02	6E-05	1.2	15
ToCP	6E-06	1E-04	2E-07	2E-03	17
TMP	6E-02	7E-05	9E-03	3.3	10
TnBP	2E-03	7E-03	6E-07	7E-04	17
TmCP	6E-06	2E-04	4E-08	4E-04	17
TpCP	6E-06	1E-04	1E-07	1E-03	17
TPhP	1E-02	4E-05	7E-04	11	5.8
T2iPPP	1E-08	3E-05	1E-09	3E-03	17
TTBNPP	2E-13	4E-05	0.0	1E-02	17
TTBPP	6E-10	7E-07	3E-11	1E-02	17
TXP	2E-04	2E-04	5E-06	11	1E-03

Table S4: Sensitivity [%] of the predicted persistence (CTD) of OPEs to a change by a factor of 1.1 of individual input parameters; Sensitivities of > 0.1% are marked green.

	Sensitivity to individual input parameters				
Chemical	Log K_{AW}	Log K_{OW}	$t_{1/2}$ air	$t_{1/2}$ water	$t_{1/2}$ soil
BCMP-BCEP	1E-10	7E-06	3E-13	9.6	9E-09
BDCPP	2E-07	3E-07	4E-10	9.6	2E-06
BEHP	2E-02	3E-02	3E-06	9.6	8E-06
BMPPP	7E-02	9E-02	1E-02	2E-04	1E-05
BPA-BDPP	8E-03	1E-02	2E-03	3E-04	1E-06
BPDP	4E-02	5E-02	6E-03	3E-04	4E-06
DCP	2E-02	2E-02	4E-02	2E-04	3E-05
DOPO	4E-02	3E-05	5E-02	5E-04	2E-03
EHDPP	0.54	5E-02	3E-06	4E-07	2E-07
IDDPP	7E-02	0.13	3E-02	0.79	8E-03
MC 984	3E-03	2E-02	1E-04	3E-05	1E-05
PBDMPP	1E-10	7E-07	1E-12	8E-13	2E-14
PBDPP	3E-04	6E-03	2E-05	5E-07	3E-09
IPPP	1E-03	3E-03	1E-04	9E-06	1E-08
TBOEP	6E-07	0.40	2E-10	9.6	1E-07
TCEP	4E-04	2E-07	8E-06	9.6	1E-04
TCIPP	3E-04	2E-06	3E-06	9.6	8E-04
TCP	3E-02	4E-02	1E-02	2E-04	3E-07
TDBPP	2E-08	5E-02	9E-13	2.4	2E-09
TDCIPP	5E-05	8E-05	8E-07	9.6	1E-03
TDMPP	1E-02	2E-02	5E-04	7E-05	8E-07
TEHP	8E-03	5E-02	9E-04	1E-05	8E-07
TEP	6E-03	1E-07	5E-02	2E-04	6E-04
TIBP	1E-03	3E-05	5E-02	3E-03	1E-05
TiPP	2E-03	1E-06	5E-02	7E-04	2E-04
ToCP	3E-02	4E-02	1E-02	2E-04	1E-05
TMP	7E-03	2E-09	5E-02	2E-04	1E-03
TnBP	9E-04	4E-04	5E-02	5E-04	2E-03
TmCP	7E-02	9E-02	1E-02	2E-04	1E-03
TpCP	3E-02	4E-02	1E-02	2E-04	9E-05
TPhP	1E-03	1E-03	5E-02	2E-03	1E-05
T2iPPP	9E-04	4E-03	2E-04	3E-05	4E-07
TTBNPP	7E-08	3E-04	4E-10	3E-10	5E-12
TTBPP	5E-05	4E-04	2E-05	1E-05	1E-07
TXP	5E-03	7E-03	6E-04	3E-05	4E-08

Table S5: Percent contribution of environmental half-lives (HL), log K_{OW} and log K_{AW} to the variance of persistence (P_{OV}) and characteristic travel distance (CTD) estimates in the Monte Carlo uncertainty analysis.

	P_{OV}					CTD				
Chemical	HL air	HL water	HL soil	log K_{OW}	log K_{AW}	HL air	HL water	HL soil	log K_{OW}	log K_{AW}
EHDPP			> 98%			> 90%				
TBOEP			> 98%			2%	86%		11%	
TIBP		14%	84%			77%	21%			
TnBP			> 93%			87%	12%			
TPhP		52%	48%			> 96%				
TCEP		>95%				22%	70%	2%		6%
TCIPP	2%	37%	16%	44%	1%	22%	70%	2%		6%
TDCIPP	2%	5%	73%	20%			> 97%			

Table S6: Result dispersion factors from the Monte Carlo uncertainty analysis for persistence (P_{OV}) and characteristic travel distance (CTD) estimates.

Chemical	P_{OV}	CTD
EHDPP	7.9	6.0
TBOEP	7.0	5.4
TIBP	6.6	7.3
TnBP	7.1	8.1
TPhP	5.5	6.4
TCEP	6.8	7.3
TCIPP	3.3	7.6
TDCIPP	7.3	5.2

Table S7: 5th percentile, median and 95th percentile of persistence (P_{OV}) and characteristic travel distance (CTD) estimates based on the Monte Carlo uncertainty analysis.

	POV			CTD		
Chemical	5th	Median	95th	5th	Median	95th
EHDPP	471	3142	15888	68	307	1137
TBOEP	31	156	700	22	75	353
TIBP	12	56	257	19	78	334
TnBP	68	333	2117	19	76	372
TPhP	23	78	397	98	500	1907
TCEP	60	125	712	77	259	1208
TCIPP	235	570	1845	93	343	1980
TDCIPP	500	1713	7716	95	505	2636

Table S8: Predicted P_{OV} [days] and LRTP in characteristic travel distance in air (CTD) [km] for OPEs at the default wind speed in the Tool (4 m s^{-1}) and the increased Arctic Oscillation wind speed (8 m s^{-1}).

Chemical	P_{OV} air	CTD air 4 m s^{-1} wind speed	CTD air 8 m s^{-1} wind speed
BCMP-BCEP	495	8.8	18
BDCPP	515	2.2	4.4
BEHP	58	346	693
BMPPP	28	562	1125
BPA-BDPP	85	2012	4024
BPDP	39	989	1977
DCP	21	369	739
DOPO	27	536	1072
EHDPP	45	234	468
IDDPP	56	231	461
MC 984	978	1526	3052
PBDMPP	432	2861	5722
PBDPP	78	2384	4768
PIP	71	2745	5490
TBOEP	63	41	83
TCEP	36	179	358
TCIPP	61	117	234
TCP	25	954	1907
TDBPP	112	139	278
TDCIPP	575	107	214
TDMPP	89	1968	3937
TEHP	49	1475	2950
TEP	0.70	70	139
TIBP	0.43	67	134
TiPP	0.48	57	114
ToCP	55	977	1954
TMP	6.2	549	1097
TnBP	0.49	67	133
TmCP	213	602	1204
TpCP	106	977	1954
TPhP	7.0	437	875
T2iPPP	136	2739	5478
TTBNPP	423	2851	5702
TTBPP	340	2853	5706
TXP	60	2412	4824

Table S9: Predicted P_{OV} [days] and LRTP in characteristic travel distance in air (CTD) [km] for OPEs at the default, global, water mass in the Tool (71%) and the reduced, continental, water mass (10%).

Chemical	P_{OV} air	CTD air 71% water	CTD air 10% water
BCMP-BCEP	495	8.8	438
BDCPP	515	2.2	868
BEHP	58	346	459
BMPPP	28	562	581
BPA-BDPP	85	2012	2038
BPDP	39	989	1011
DCP	21	369	395
DOPO	27	536	603
EHDPP	45	234	242
IDDPP	56	231	237
MC 984	978	1526	1527
PBDMPP	432	2861	2861
PBDPP	78	2384	2384
PIP	71	2745	2747
TBOEP	63	41	47
TCEP	36	179	222
TCIPP	61	117	333
TCP	25	954	999
TDBPP	112	139	148
TDCIPP	575	107	437
TDMPP	89	1968	1977
TEHP	49	1475	1481
TEP	0.70	70	71
TIBP	0.43	67	68
TiPP	0.48	57	58
ToCP	55	977	1023
TMP	6.2	549	621
TnBP	0.49	67	68
TmCP	213	602	619
TpCP	106	977	1023
TPhP	7.0	437	478
T2iPPP	136	2739	2745
TTBNPP	423	2851	2851
TTBPP	340	2853	2853
TXP	60	2412	2416

Table S10: Predicted P_{OV} [days] and LRTP in characteristic travel distance in water (CTD) [km] for OPEs at the default, marine, flow velocity in the Tool (0.02 m s^{-1}) and the increased, river-based, flow rate (0.02 m s^{-1}).

Chemical	P_{OV} air	P_{OV} water	CTD air	CTD water 0.02 m s^{-1} flow	CTD water 0.04 m s^{-1} flow
BCMP-BCEP	495	260	8.8	446	866
BDCPP	515	527	2.2	897	1744
BEHP	58	399	346	601	1168
BMPPP	28	55	562	93	181
BPA-BDPP	85	87	2012	112	218
BPDP	39	55	989	87	170
DCP	21	54	369	93	181
DOPO	27	54	536	93	181
EHDPP	45	47	234	80	155
IDDPP	56	134	231	215	418
MC 984	978	260	1526	424	825
PBDMPP	432	260	2861	121	236
PBDPP	78	55	2384	91	176
PIP	71	87	2745	79	155
TBOEP	63	27	41	47	92
TCEP	36	130	179	225	437
TCIPP	61	196	117	338	656
TCP	25	55	954	92	180
TDBPP	112	87	139	149	290
TDCIPP	575	260	107	445	866
TDMPP	89	55	1968	72	139
TEHP	49	14	1475	22	42
TEP	0.70	22	70	37	73
TIBP	0.43	21	67	36	69
TiPP	0.48	21	57	37	72
ToCP	55	55	977	92	180
TMP	6.2	22	549	37	73
TnBP	0.49	12	67	21	42
TmCP	213	55	602	92	180
TpCP	106	55	977	92	180
TPhP	7.0	47	437	82	159
T2iPPP	136	55	2739	62	120
TTBNPP	423	260	2851	139	270
TTBPP	340	260	2853	121	236
TXP	60	87	2412	87	169

Table S11: Change in CTD at doubled wind speed and flow velocity, respectively, compared to the default Tool settings.

	Double wind speed		Double flow velocity	
Chemical	ΔCTD_{air}	ΔCTD_{water}	ΔCTD_{air}	ΔCTD_{water}
BCMP-BCEP	2.0	1.0	1.0	1.94
BDCPP	2.0	1.0	1.0	1.94
BEHP	2.0	1.0	1.0	1.94
BMPPP	2.0	1.0	1.0	1.94
BPA-BDPP (BADP)	2.0	1.0	1.0	1.95
BPDP	2.0	1.0	1.0	1.95
DCP	2.0	1.0	1.0	1.94
DOPO	2.0	1.0	1.0	1.94
EHDPP	2.0	1.0	1.0	1.95
IDDPP	2.0	1.0	1.0	1.95
MC 984	2.0	1.0	1.0	1.94
PBDMPP	2.0	1.0	1.0	1.95
PBDPP	2.0	1.0	1.0	1.94
PIP	2.0	1.0	1.0	1.95
TBOEP	2.0	1.0	1.0	1.94
TCEP	2.0	1.0	1.0	1.95
TCIPP	2.0	1.0	1.0	1.94
TCP	2.0	1.0	1.0	1.95
TDBPP	2.0	1.0	1.0	1.94
TDCIPP	2.0	1.0	1.0	1.94
TDMPP	2.0	1.0	1.0	1.94
TEHP	2.0	1.0	1.0	1.93
TEP	2.0	1.0	1.0	1.96
TIBP	2.0	1.0	1.0	1.94
TiPP	2.0	1.0	1.0	1.94
TmCP	2.0	1.0	1.0	1.95
TMP	2.0	1.0	1.0	1.96
TnBP	2.0	1.0	1.0	1.96
ToCP	2.0	1.0	1.0	1.95
TpCP	2.0	1.0	1.0	1.95
TPhP	2.0	1.0	1.0	1.95
T2iPPP	2.0	1.0	1.0	1.94
TTBNPP	2.0	1.0	1.0	1.94
TTBPP	2.0	1.0	1.0	1.94
TXP	2.0	1.0	1.0	1.94