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

A Framework to Model Exposure to Per- and Polyfluoroalkyl Substances in Indoor Environments

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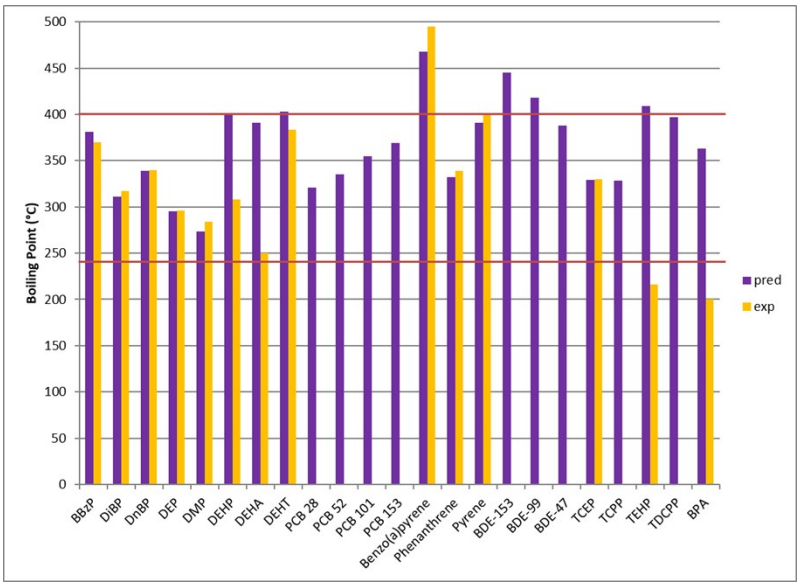

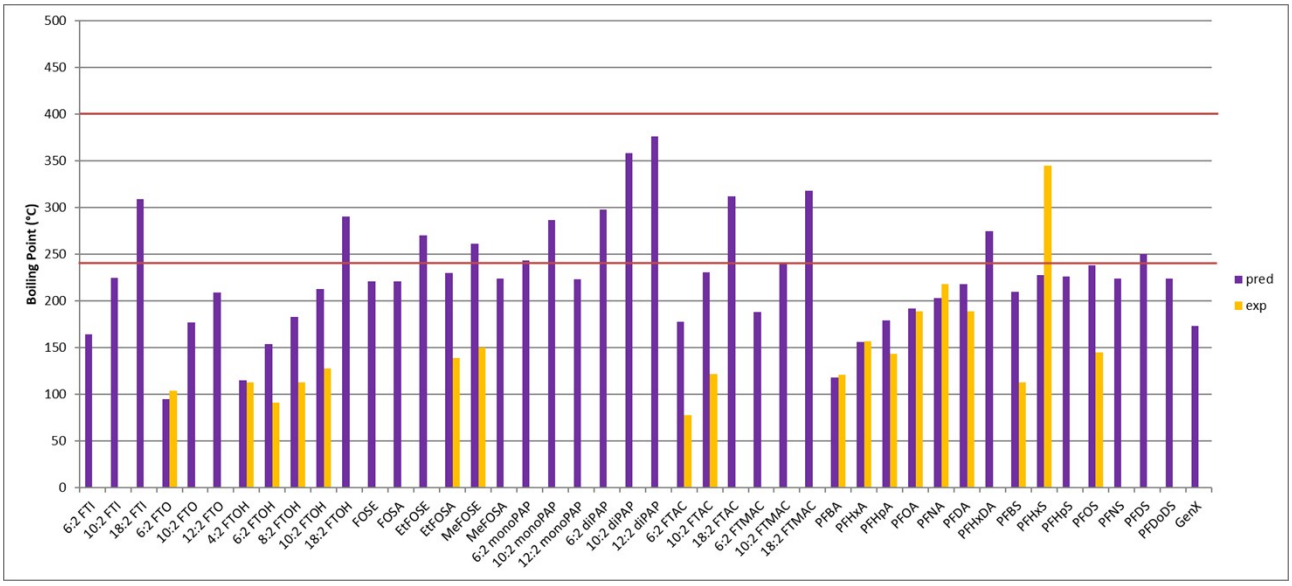

Figure S1: Predicted (pred) and experimental (exp) average vapor pressures and boiling points of selected SVOCs (top) and PFAS (bottom) compounds, as listed by the US EPA CompTox Chemistry Dashboard[1]. Red lines indicate the definition range for SVOCs according to the WHO[2] based on boiling point.

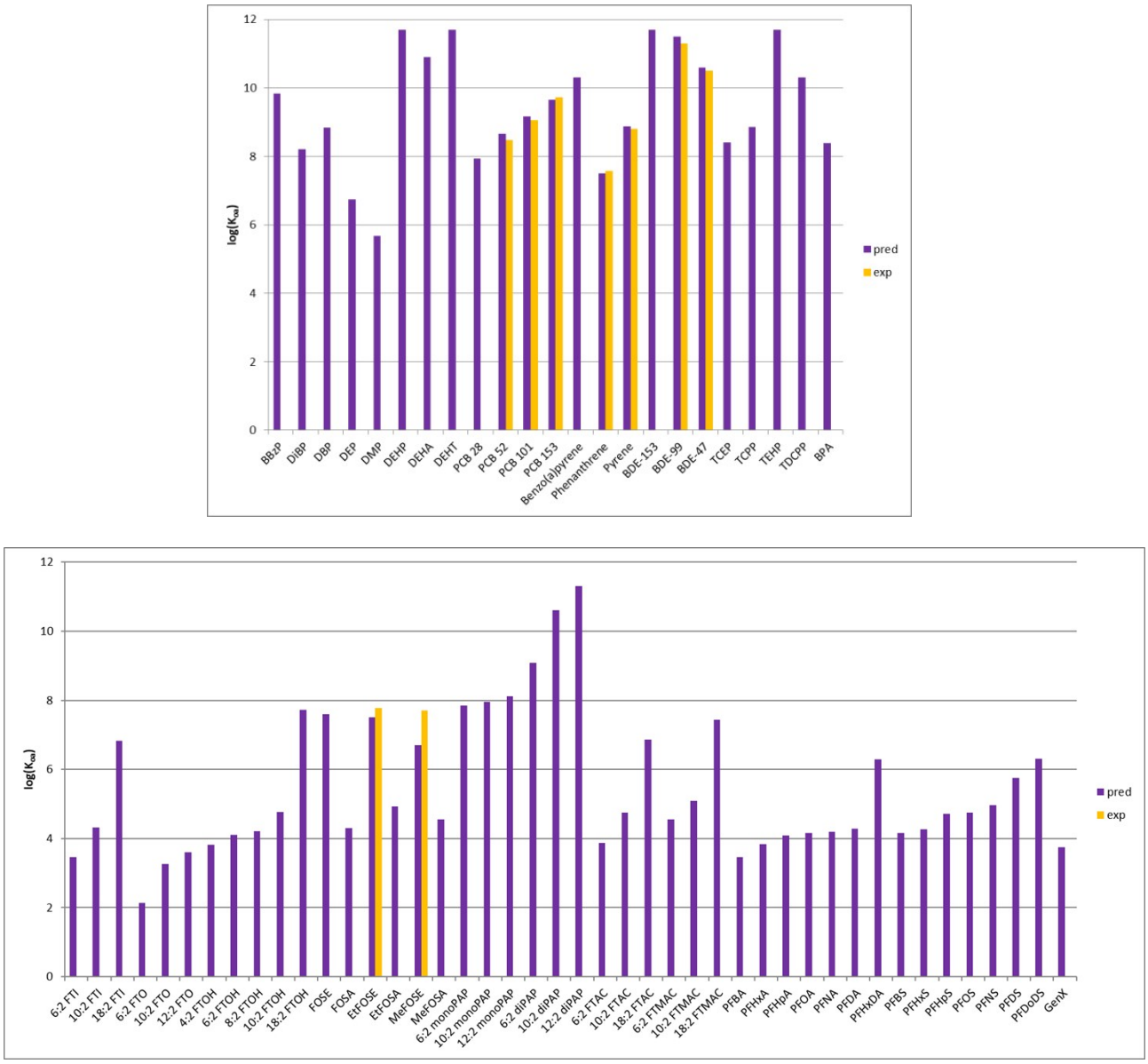

Figure S2: Predicted (pred) and experimental (exp) average log(K_{oa}) values of selected SVOCs (top) and PFAS (bottom) compounds,

as listed by the US EPA CompTox Chemistry Dashboard[1].

Table S1: Chemical properties of selected PFAS[1]

	Compound		CASRN	MW (g/mol)	log(K_{ow})		Boiling Point (°C)		Water solubility (mol/L)		Vapor pressure (Pa)		Density (g/cm^3)		Henry's Law (atm-m^3/mole)		log(K_{oa})	
					exp avg	pred avg	exp avg	pred avg	exp avg	pred avg	exp avg	pred avg	exp avg	pred avg	exp avg	pred avg	exp avg	pred avg
PFAA precursors	Fluorotelomer iodides	6:2 FTI	2043-57-4	474.0		6.33		164		4.02E-06		1.3E+02		1.94		1.12E-03		3.46
		10:2 FTI	2043-54-1	674.0		8.70		225		7.52E-07		1.1E+03		1.96		5.81E-06		4.32
		18:2 FTI	65104-63-4	1074.1		13.90		309		6.64E-07		6.9E-04		2.20		1.02E-08		6.83
	Fluorotelomer olefins	6:2 FTO	25291-17-2	346.1		5.28	104	94.6		2.21E-05		9.2E+03		1.52		1.11E-02		2.13
		10:2 FTO	30389-25-4	546.1		8.15		177		5.97E-07		1.4E+03		1.69		6.18E-06		3.26
		12:2 FTO	67103-05-3	646.1		8.58		209		1.58E-06		6.4E+02		1.70		3.77E-08		3.6
	Fluorotelomer alcohols	4:2 FTOH	2043-47-2	264.1	3.30	2.95	113	115	3.67e-4	1.14E-02	1.2E+03	2.2E+03		1.51		2.67E-09		3.82
		6:2 FTOH	647-42-7	364.1	4.54	4.56	91.1	154	4.60e-5	8.55E-04	3.7E+02	2.5E+02		1.56		2.76E-10		4.1
		8:2 FTOH	678-39-7	464.1	5.58	6.06	113	183	4.20e-7	5.56E-05	1.6E+00	1.5E+01		1.59		2.17E-10		4.22
		10:2 FTOH	865-86-1	564.1		7.49	128	213		7.63E-06	1.4E+02	3.2E+00		1.67		3.95E-10		4.76
		18:2 FTOH	65104-65-6	964.2		12.00		290		6.44E-06		4.6E-04		1.95		1.29E-09		7.72
	Perfluorooctane sulfonamidoethanol	FOSE	10116-92-4	543.2		3.59		221		5.27E-06		1.6E-01				1.61E-11		7.6
	Perfluorooctane sulfonamide	FOSA	754-91-6	499.1		5.95		221		7.72E-06	3.3E+01	4.5E+01		1.79		1.33E-09		4.3
	N-Ethyl perfluorooctane sulfonamidoethanol	EtFOSE	1691-99-2	571.3		6.31		270	2.64e-7	5.28E-04		2.7E+00		1.71		3.52E-10	7.78	7.5
	N-Ethyl perfluorooctane sulfonamide	EtFOSA	4151-50-2	527.2		6.25	139	230		3.36E-05	5.7E-05	1.9E+01		1.63		1.67E-10		4.92
	N-Methyl perfluorooctane sulfonamidoethanol	MeFOSE	24448-09-7	557.2		5.94	150	261		6.05E-04	2.0E-03	3.9E+00		1.73		3.55E-10	7.70	6.71
	N-Methyl perfluorooctane sulfonamide	MeFOSA	31506-32-8	513.2		6.07		224		7.70E-06		3.2E+01		1.66		1.69E-10		4.56
	Polyfluoroalkyl phosphoric acid monoesters	6:2 monoPAP	57678-01-0	444.1		3.24		243		5.38E-04		4.7E-02		1.74		1.50E-11		7.84
		10:2 monoPAP	57678-05-4	644.1		6.02		287		2.41E-05		2.7E-03		2.00		1.59E-11		7.96
		12:2 monoPAP	57678-07-6	744.1		5.20		223		1.37E-05		1.2E-01				1.38E-11		8.11
	Polyfluoroalkyl phosphoric acid diesters	6:2 diPAP	57677-95-9	790.2		7.30		298		9.97E-07		6.9E-04		1.89		1.48E-11		9.08
		10:2 diPAP	1895-26-7	1190.2		13.20		358		7.48E-07		1.3E-07		2.41		1.36E-10		10.6
		12:2 diPAP	57677-99-3	1390.3		15.80		376		7.70E-07		8.0E-08		2.57		6.90E-10		11.3
	Fluorotelomer acrylates	6:2 FTAC	17527-29-6	418.15	5.20	5.66	78	178	9.09e-7	6.93E-04	4.4E+01	6.2E+03		1.54		6.19E-06		3.87
		10:2 FTAC	17741-60-5	618.2		7.99	122	231		2.61E-05		2.7E+01		1.71		1.49E-08		4.75
		18:2 FTAC	65104-64-5	1018.2		13.20		312		1.22E-07		3.7E-04		1.92		1.03E-08		6.87
	Fluorotelomer methacrylates	6:2 FTMAC	2144-53-8	432.2		5.99		188		7.54E-05		1.9E+01		1.56		2.63E-07		4.56
		10:2 FTMAC	2144-54-9	632.2		8.50		240		5.66E-07		4.5E+00		1.70		2.68E-07		5.09
		18:2 FTMAC	65104-66-7	1032.3		13.70		318		1.04E-07		1.3E-04		1.90		1.03E-08		7.44
PFCAs	Perfluorobutanoic acid	PFBA	375-22-4	214.0	1.43	2.71	121	118	2.09e-3	7.34E-03	8.5E+02	7.7E+02	1.65	1.61		4.99E-05		3.46
	Perfluorohexanoic acid	PFHxA	307-24-4	314.1	2.51	3.94	157	156	9.39e-5	3.54E-04	1.2E+02	1.9E+02		1.69		2.51E-10		3.83
	Perfluoroheptanoic acid	PFHpA	375-85-9	364.1		4.49	143	179	0.324	6.34E-04	7.3E+01	4.3E+01		1.71		2.22E-10		4.09
	Perfluorooctanoic acid	PFOA	335-67-1	414.1	3.60	5.51	189	192	1.56e-2	1.01E-02	3.0E+02	3.3E+01	1.80	1.72		2.02E-10		4.16
	Perfluorononanoic acid	PFNA	375-95-1	464.1		6.18	218	203		1.00E-03		1.0E+01		1.78		1.64E-10		4.2
	Perfluorodecanoic acid	PFDA	335-76-2	514.1		6.89	189	218		2.94E-03		4.1E+00		1.79		3.55E-10		4.28
	Perfluorohexadecanoic acid	PFHxDA	67905-19-5	814.1		10.80		275		8.20E-06		6.7E-01		1.89		3.85E-10		6.29

	Compound		CASRN	MW (g/mol)	log(K_{ow})		Boiling Point (°C)		Water solubility (mol/L)		Vapor pressure (Pa)		Density (g/cm^3)		Henry's Law ($atm\text{-}m^3$/mole)		log(K_{oa})	
PFSAs	Perfluorobutane sulfonic acid	PFBS	375-73-5; 59933-66-3	300.1		1.98	113	210	1.70e-3	2.41E-02		3.2E+01		1.83		3.04E-10		4.16
	Perfluorohexane sulfonic acid	PFHxS	355-46-4	400.1	2.20	3.44	345	228	6.08e-4	3.36E-04	1.1E-06	1.3E+00		1.84		1.96E-10		4.27
	Perfluoroheptane sulfonic acid	PFHpS	375-92-8	450.1		4.06		226		3.63E-04		1.5E+00		1.86		2.34E-10		4.71
	Perfluorooctane sulfonic acid	PFOS	1763-23-1	500.1		4.05	145	238		2.79E-04	3.3E-04	1.0E+00		1.84		1.85E-11		4.75
	Perfluorononane sulfonic acid	PFNS	474511-07-4	549.1		1.68		224		4.04E-04		1.5E+00				1.88E-11		4.97
	Perfluorodecane sulfonic acid	PFDS	335-77-3	600.1		5.81		250		8.44E-05		6.3E-01		1.88		3.46E-10		5.76
	Perfluorododecane sulfonic acid	PFDoDS	79780-39-5	700.2		4.58		224		3.96E-05		1.3E+00				3.59E-10		6.30
PFEAs	Ammonium perfluoro-2-methyl-3-oxahexanoate	GenX	62037-80-3	347.0		1.98		173		5.31E-04		5.52E-02				2.37E-10		3.74

Table S2: Chemical properties of selected SVOCs[1]

	Compound		CASRN	MW (g/mol)	log(K_{ow})		Boiling Point (°C)		Water solubility (mol/L)		Vapor pressure (Pa)		Density (g/cm³)		Henry's Law (atm-m³/mole)		log(K_{oa})	
					exp avg	pred avg	exp avg	pred avg	exp avg	pred avg	exp avg	pred avg	exp avg	pred avg	exp avg	pred avg	exp avg	pred avg
Phthalate esters	Benzyl butyl phthalate	BBzP	85-68-7	312.4	4.73	4.57	370	381	8.61E-06	1.88E-05	1.1E-03	6.9E-04		1.13		2.82E-08		9.83
	Diisobutyl phthalate	DiBP	84-69-5	278.3	4.11	4.26	317	311	2.23E-05	5.36E-05		5.4E-02		1.04		3.13E-07		8.21
	Dibutyl phthalate	DBP	84-74-2	278.3	4.50	4.60	340	339	4.02E-05	3.23E-05	2.7E-03	5.9E-03		1.05	1.81E-06	1.20E-06		8.84
	Diethyl phthalate	DEP	84-66-2	222.2	2.42	2.54	296	295	4.86E-03	3.06E-03	2.8E-01	2.2E-01		1.12		2.38E-08		6.75
	Dimethyl phthalate	DMP	131-11-3	194.2	1.60	1.66	284	273	2.06E-02	1.25E-02	4.1E-01	5.0E-01		1.15		9.36E-08		5.68
	Diethylhexyl phthalate	DEHP	117-81-7	390.6	7.60	8.00	308	399	1.08E-07	8.79E-07	1.9E-05	1.6E-04		0.97		2.60E-07		11.70
Phthalate alternatives	Bis(2-ethylhexyl) adipate	DEHA	103-23-1	370.6			250	391	2.10E-06	2.23E-06	1.1E-04	4.5E-04		0.91	4.34E-07	4.11E-07		10.90
	Bis(2-ethylhexyl) terephthalate	DEHT	6422-86-2	390.6		8.14	383	403		4.55E-07		1.2E-04		0.97		2.57E-07		11.70
PCBs	2,4,4'-Trichlorobiphenyl	PCB 28	7012-37-5	257.5	5.62	5.53		321	1.05E-06	1.15E-06	1.9E-02	1.7E-01		1.34	2.00E-04	1.94E-04		7.93
	2,2',5,5'-Tetrachlorobiphenyl	PCB 52	35693-99-3	292.0	6.09	5.93		335	5.24E-08	3.63E-07	3.4E-03	9.3E-03		1.42	2.00E-04	1.78E-04	8.47	8.65
	2,2',4,5,5'-Pentachlorobiphenyl	PCB 101	37680-73-2	326.4	5.68	6.40		355	4.72E-08	7.62E-08	2.1E-03	2.7E-03		1.52	9.00E-05	8.39E-05	9.06	9.16
	2,2',4,4',5,5'-Hexachlorobiphenyl	PCB 153	35065-27-1	360.9	6.34	6.92		369	2.63E-09	1.15E-08	2.7E-04	6.6E-04		1.60	2.30E-05	2.93E-05	9.73	9.66
PAHs	Benzo(a)pyrene		50-32-8	252.3	6.13	5.92	495	468	6.42E-09	3.54E-08		7.3E-07	1.6E-05	1.28	4.57E-07	5.71E-07		10.30
	Phenanthrene		85-01-8	178.2	4.46	4.32	339	332	6.45E-06	3.18E-06		1.6E-02	1.4E-02	1.12	4.23E-05	5.18E-05	7.57	7.50
	Pyrene		129-00-0	202.3	4.88	4.83	399	391	6.67E-07	5.48E-07		6.0E-04	2.9E-04	1.24	1.19E-05	1.16E-05	8.80	8.87
Flame retardants	2,2',4,4',5,5'-Hexabromodiphenyl ether	BDE-153	68631-49-2	643.6	7.90	7.91		445		4.22E-09		1.9E-06		2.68		1.09E-05		11.70
	2,2',4,4',5-Pentabromodiphenyl ether	BDE-99	60348-60-9	564.7	7.32	7.21		418		2.73E-08	4.1E-06	1.1E-05		2.46		1.09E-05	11.30	11.50
	2,2',4,4'-Tetrabromodiphenyl ether	BDE-47	5436-43-1	485.8	6.81	6.50		388		9.44E-08	9.3E-06	1.6E-04		2.26		1.02E-05	10.50	10.60
	Tris(2-carboxyethyl)phosphine	TCEP	115-96-8	285.5	1.44	1.32	330	329	2.45E-02	9.66E-03	8.2E+00	2.3E+00		1.41		1.28E-07		8.41
	Tris(2-chloroisopropyl)phosphate	TCPP	13674-84-5	327.6	2.59	2.43		328	3.66E-03	1.12E-03		5.9E-01		1.30		1.58E-06		8.85
	Tris(2-ethylhexyl) phosphate	TEHP	78-42-2	434.6		8.77	216	409		3.21E-06	1.1E-05	2.0E-04		0.90		2.41E-06		11.70
	Tris(1,3-dichloroisopropyl)-phosphate	TDCPP	13674-87-8	430.9	3.65	3.12		397	1.62E-05	6.10E-05		3.5E-03		1.52		1.68E-06		10.30
Phenols	Bisphenol A	BPA	80-05-7	228.3	3.32	3.29	200	363	5.26E-04	9.62E-04		1.1E-04		1.17		1.26E-07		8.38

References

1. USEPA, CompTox Chemistry Dashboard, https://www.epa.gov/chemical-research/chemistry-dashboard, (accessed Nov 14, 2019).
2. WHO, *Indoor air quality: organic pollutants*, World Health Organization, Copenhagen, NL, 1989.