RoTS verification

G D

17 July, 2021

Raw data used

The raw data used consists of a limited dataset of 26 samples, 13 “schudproeven” (SP) and 13 “kolomproeven” (KP). Data is lifted from Table 10 (p.22 and 23) of memo OWV7-ATL-NOT-013.

Schudproef / kolomproef	monster nummer	Uitloging (μg/l)	Concentratie gidsparameter (μg/kg ds)
SP	B60001	23.00	88
SP	B60002	29.00	85
SP	B60003	1.60	13
SP	B60007	57.00	551
SP	B60008	46.00	551
SP	B60101	8.80	490
SP	B60102	3.30	217
SP	B60104	4.10	217
SP	MM50201-205	0.45	10
SP	MM50207-208	0.34	21
SP	MM50301-303	0.22	13
SP	MM50306-307	0.25	15
SP	B70004KP	9.20	67
KP	B60001	28.00	88
KP	B60002	20.00	85
KP	B60003	1.20	13
KP	B60007	49.00	551
KP	B60008	44.00	551
KP	B60101	13.00	490
KP	B60102	4.60	217
KP	B60104	3.20	217
KP	MM50201-205	0.39	10
KP	MM50207-208	0.42	21
KP	MM50301-303	0.42	13
KP	MM50306-307	0.46	15
KP	B70004KP	5.90	67

Summary statistics full dataset

Note the inconsistencies with values reported in the original memo where the mean “gidsparameter” value is set to be 152.08 rather than 179.85.

Summary statistic	Uitloging (μg/l)	Concentratie gidsparameter (μg/kg ds)
mean	13.61	179.85
median	4.35	85.00
min	0.22	10.00
max	57.00	551.00

Summary statistics limited dataset

The limited dataset consists of all samples with "uitloging" concentrations of less than 10μg/l.

Summary statistic	Uitloging (μg/l)	Concentratie gidsparameter (μg/kg ds)
mean	2.64	96.24
median	1.20	21.00
min	0.22	10.00
max	9.20	490.00

Empirical model fits as reported

Schudproef / Kolomproef (or combined)	set (limited <10 μg/l uitloging)	a	b	R2	functional form
KP	full	28.289	0.5802	0.65	power
SP	full	32.497	0.6230	0.68	power
KP + SP	full	30.263	0.6026	0.66	power
KP	full	35.513	0.0431	0.30	exp
SP	full	34.401	0.0540	0.45	exp
KP + SP	full	34.730	0.0492	0.38	exp
KP	limited	29.344	0.9360	0.73	power
SP	limited	35.649	0.8102	0.68	power
KP + SP	limited	32.467	0.8572	0.70	power
KP	limited	12.722	0.4703	0.65	exp
SP	limited	16.989	0.3132	0.57	exp
KP + SP	limited	15.710	0.3494	0.58	exp

Empirical model fits as calculated

Data were fit using an exponential and power curve, on both SP and KP groups separately or combined. Assuming processing using a spreadsheet linearized (log transformed) data was used to estimate parameters a and b for both functional forms.

Schudproef / Kolomproef (or combined)	set (limited <10 μg/l uitloging)	a	b	R2	functional form
KP	full	28.0470	0.7064	0.74	power
SP	full	32.4973	0.6230	0.68	power
KP + SP	full	30.3667	0.6612	0.70	power
KP	full	32.0960	0.0633	0.50	exp
SP	full	34.4012	0.0540	0.45	exp
KP + SP	full	33.3947	0.0581	0.47	exp
KP	limited	29.3437	0.9360	0.73	power

Schudproef / Kolomproef (or combined)	set (limited <10 μg/l uitloging)	a	b	R2	functional form
SP	limited	35.6489	0.8102	0.68	power
KP + SP	limited	32.4666	0.8572	0.70	power
KP	limited	12.7225	0.4703	0.65	exp
SP	limited	16.9893	0.3132	0.57	exp
KP + SP	limited	15.7100	0.3494	0.58	exp

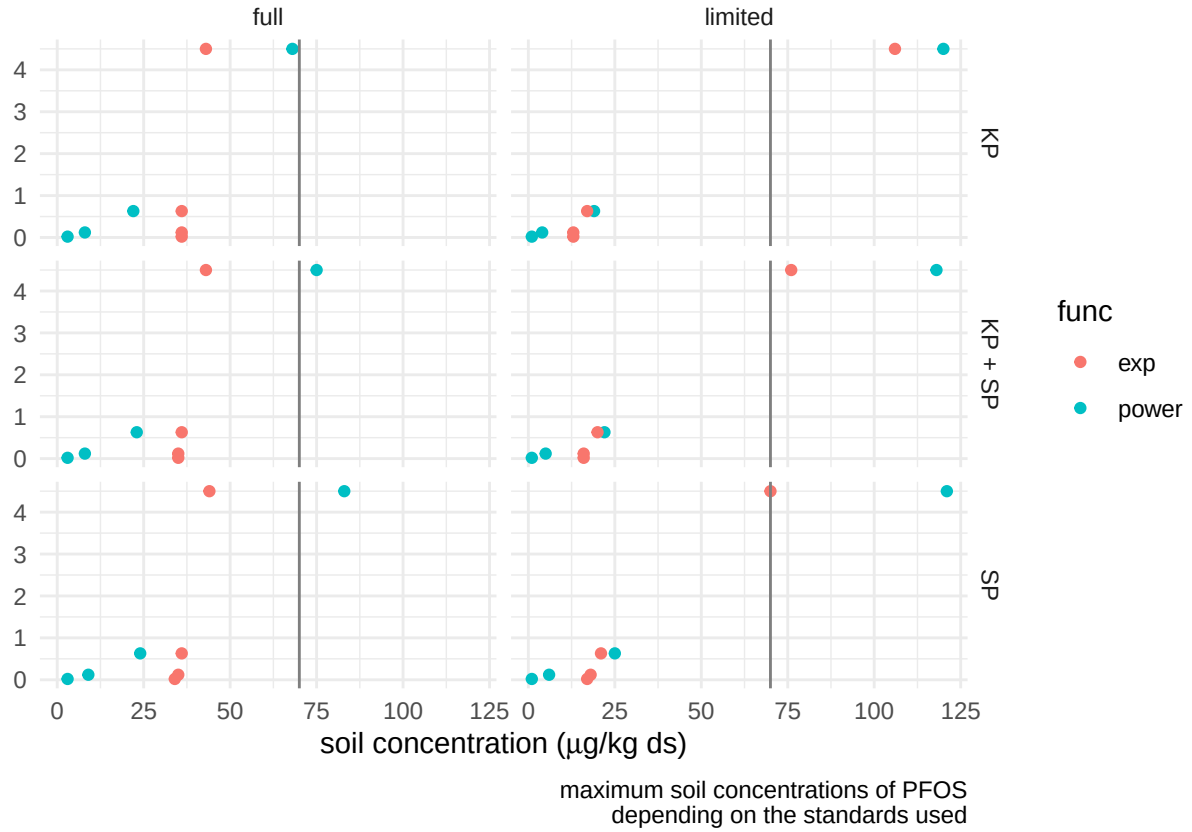
Differences in model fits

Differences in parameters between recalculated fits and reported values are minimal, can be attributed to rounding errors and small mis-reporting of values.

Schudproef / Kolomproef (or combined)	set (limited <10 μg/l uitloging)	Δa (analysis - memo)	Δb (analysis - memo)	R2	functional form
KP	full	-0.2420	0.1262	0.09	power
SP	full	0.0003	0.0000	0.00	power
KP + SP	full	0.1037	0.0586	0.04	power
KP	full	-3.4170	0.0202	0.20	exp
SP	full	0.0002	0.0000	0.00	exp
KP + SP	full	-1.3353	0.0089	0.09	exp
KP	limited	-0.0003	0.0000	0.00	power
SP	limited	-0.0001	0.0000	0.00	power
KP + SP	limited	-0.0004	0.0000	0.00	power
KP	limited	0.0005	0.0000	0.00	exp
SP	limited	0.0003	0.0000	0.00	exp
KP + SP	limited	0.0000	0.0000	0.00	exp

Soil concentrations using the above empirical fits (memo)

Given equivalence between re-analysis data and provided parameters the provided parameters are used.



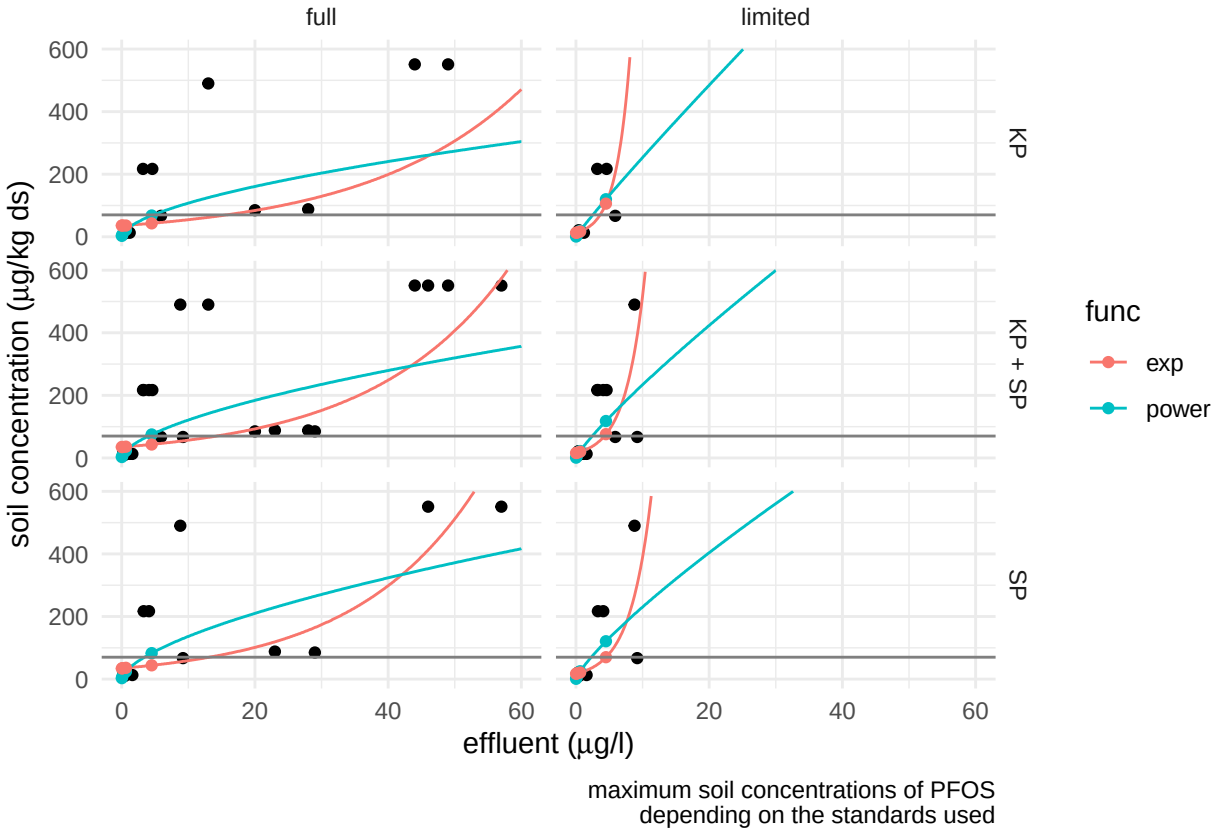
Model selection

Standard model selection using an AIC (all are linear models so only dependent on residuals and number of values used).

Schudproef / Kolomproef (or combined)	set (limited <10 μg/l uitloging)	R2	AIC	functional form	Soil concentration (μg/kg ds)
KP	limited	0.73	21.11	power	120
KP	limited	0.65	23.29	exp	106
SP	limited	0.68	27.58	power	121
SP	limited	0.57	30.18	exp	70
KP	full	0.74	35.54	power	81
SP	full	0.68	38.32	power	83
KP + SP	limited	0.70	43.65	power	118
KP	full	0.50	43.95	exp	43
SP	full	0.45	45.21	exp	44
KP + SP	limited	0.58	48.96	exp	76
KP + SP	full	0.70	68.26	power	82
KP + SP	full	0.47	83.36	exp	43
KP	limited	0.44	95.23	lin	139
SP	limited	0.47	116.54	lin	160
KP	full	0.58	169.93	lin	98
SP	full	0.52	171.73	lin	103
KP + SP	limited	0.48	208.41	lin	153

Schudproef / Kolomproef (or combined)	set (limited <10 μg/l uitloging)	R2	AIC	functional form	Soil concentration (μg/kg ds)
KP + SP	full	0.54	335.95	lin	101

Full functional responses



maximum soil concentrations of PFOS depending on the standards used