

Supplementary Material

Combined leaching and plant uptake simulations of PFOS and PFOA under field conditions

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Table 4 Plant parameters used in the basic run of the MACRO model

Parameter	Description	Unit	Canola	Winter Wheat	Winter Rye	Winter barley
CFORM ^a	Form factor LAI development	-	2.0	2.0	2.0	2.0
DFORM ^a	Form factor LAI development	-	0.2	0.2	0.2	0.2
BETA ^a	Root adaptability factor	-	0.1	0.1	0.1	0.1
CANCAP ^a	Canopy interception capacity	mm	3	3	3	3
RSMIN ^a	Minimum stomatal resistance	s/m	40	50	50	50
LAIMIN ^a	Leaf are index at ZDATEMIN	-	1	1	1	1
LAIMAX	Leaf are index at IDMAX	-	5 ^a / 2.5 ^c	6 ^a	6 ^a	7 ^d
LAIHAR	Leaf area index at harvest	-	0.5 ^b	2 ^a	2 ^a	2 ^a
ROOTINIT ^a	Root depth at ZDATEMIN	m	0.2	0.2	0.2	0.2
ROOTMAX ^e	Maximum root depth	m	0.9	1.3	1.5	1.2
ZHMIN ^a	Crop height at ZDATEMIN	m	0.2	0.2	0.2	0.2
HMAX ^a	Maximum crop height	m	0.7	0.8	0.8	0.8
IDSTART	Day of crop emergence	Julian day	246	265	265	265
IDMAX	Day of maximum leaf area/root depth	Julian day	156	172	172	172
ZDATEMIN	Day of intermediate crop development	Julian day	60	77	77	77
IHARV	Day of harvest	Julian day	221	233	233	233

^aFOCUS 2012

^bDiepenbrock 2000

^cIn 2012 harvested biomass was only half of 2009, thus we assumed also only half the LAI

^destimated; barley has a higher LAI than winter wheat (Bach et al. 2016)

^eestimated in the range reported by Fan et al. (2016)

Table 5 Site Parameters

Parameter	Description	UNIT	Value
ANNTAV	Average annual temperature	°C	9.5
ANNAM	Average annual temperature amplitude	°C	9.3
SNOWMF	Snowmelt factor	mm/°C/d	4
PHI	Site latitude	°	51.3
RINTEN	Average rainfall intensity	mm/h	0.66
ALBEDO	Albedo	-	0.1
ZMET	Height of windspeed measurement	m	15

Table 6 Soil properties as measured in the lysimeter, (Heyn 2013) soil layers were combined (arithmetic average)

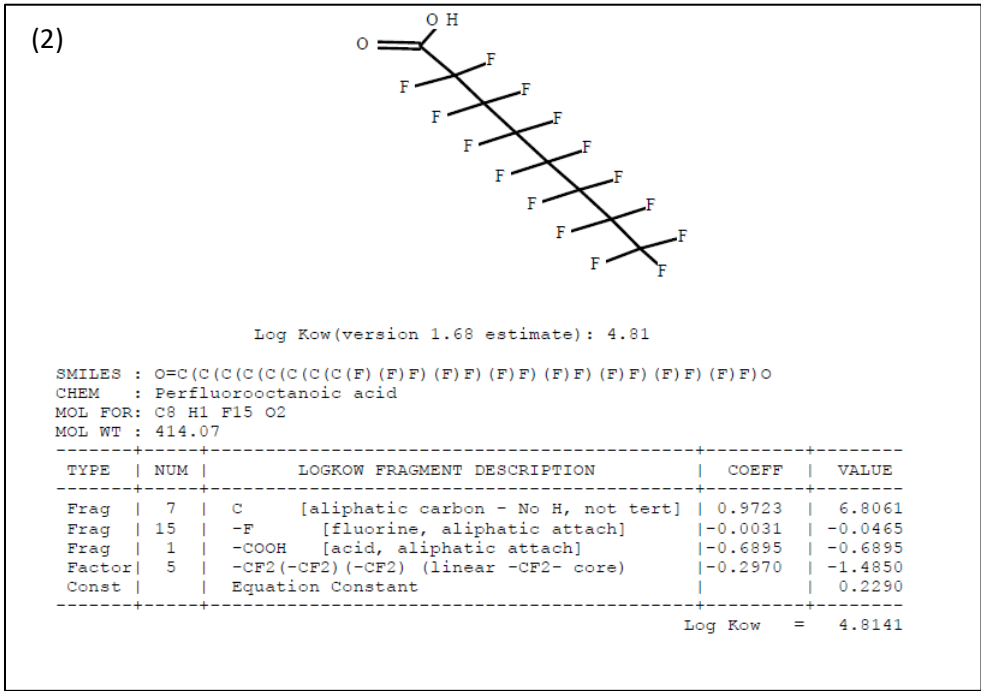
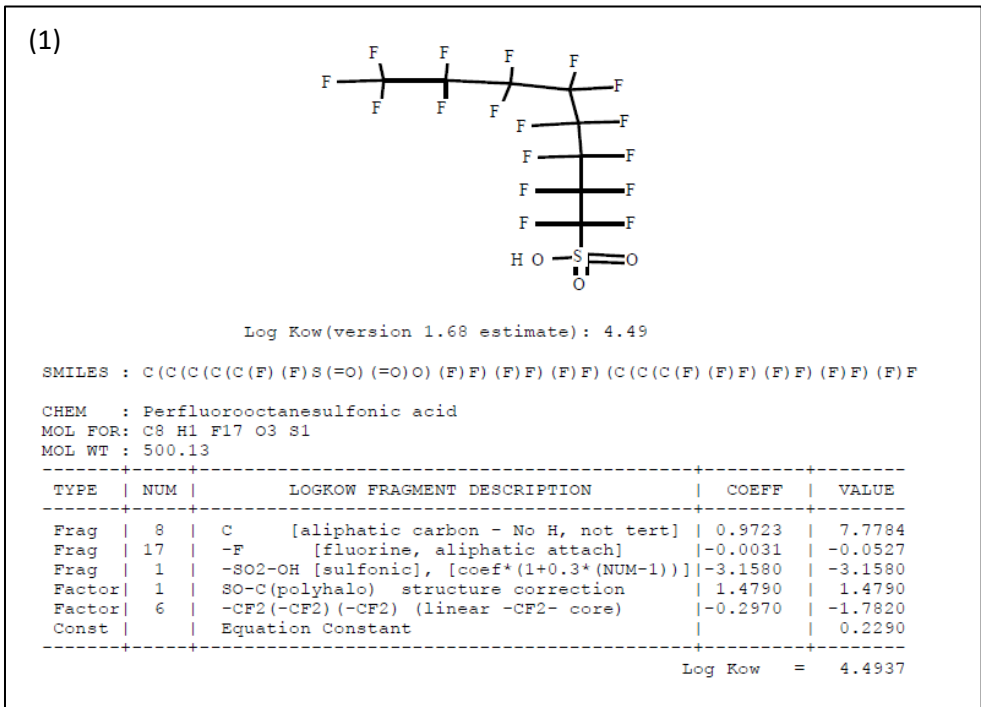
Description	Unit	Horizon Ap	Horizon B	Horizon C1	Horizon C2
Depth of soil layer	m	0.1	0.4	0.8	0.2
Clay content	%	17	18.2	26.8	23.8
Silt content	%	79.6	78.9	70.9	73.9
Sand content	%	3.4	2.9	2.3	2.3
pH	-	6.5	6.8	6.9	7.0
Organic carbon content	%	1.5	0.8	0.3	0.2
ρ_s^a	g/cm ³	1.5			

^aSoil density was assumed based on typical characteristics

61 **Table 7** Soil parameters as calculated by MACRO pedotransfer functions using soil properties from
62 Table 6.

Parameter	Description	Unit	Horizon Ap	Horizon B	Horizon C1	Horizon C2
TPORV	Saturated water content	%	42.16	42.4	42.57	42.6
XMPOR	Boundary water content	%	39.31	40.95	41.57	41.6
WILT	Wilting point	%	13.35	14.66	18.58	16.54
RESID	Residual water content	%	0	0	0	0
GAMMA	Bulk density	g/cm ³	1.5	1.5	1.5	1.5
CTEN	Boundary water tension	cm	10	10	10	10
N	van Genuchten's N	-	1.224	1.206	1.157	1.181
KSATMIN	Saturated hydraulic conductivity	mm/h	13.38	3.25	2.59	2.87
KSM	Boundary hydraulic conductivity	mm/h	0.42666	0.40283	0.29776	0.32833
ZN	Pore size distribution factor	-	4	2	6	6
ZM	Tortuosity factor (micropores)	-	0.5	0.5	0.5	0.5
ASCALE	Effective diffusion pathlength	mm	4	4	4	4
ALPHA	van Genuchten's alpha	1/cm	0.008668	0.010155	0.012599	0.011706
TRAP_AIR	Trapped air content	%	0	0	0	0

Fig. 4 Result of calculating K_{ow} for PFOS (1) and PFOA (2) with EPI Suite™



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