

Figure S1: Ratio of the individual US-EPA PAH concentration in leachates from COK1 soil under low ionic strength conditions (s) and low (t) or high (T) temperature and low (a) or high (A) availability level conditions to their respective solubilities. The dotted line corresponds to the solubility limit.

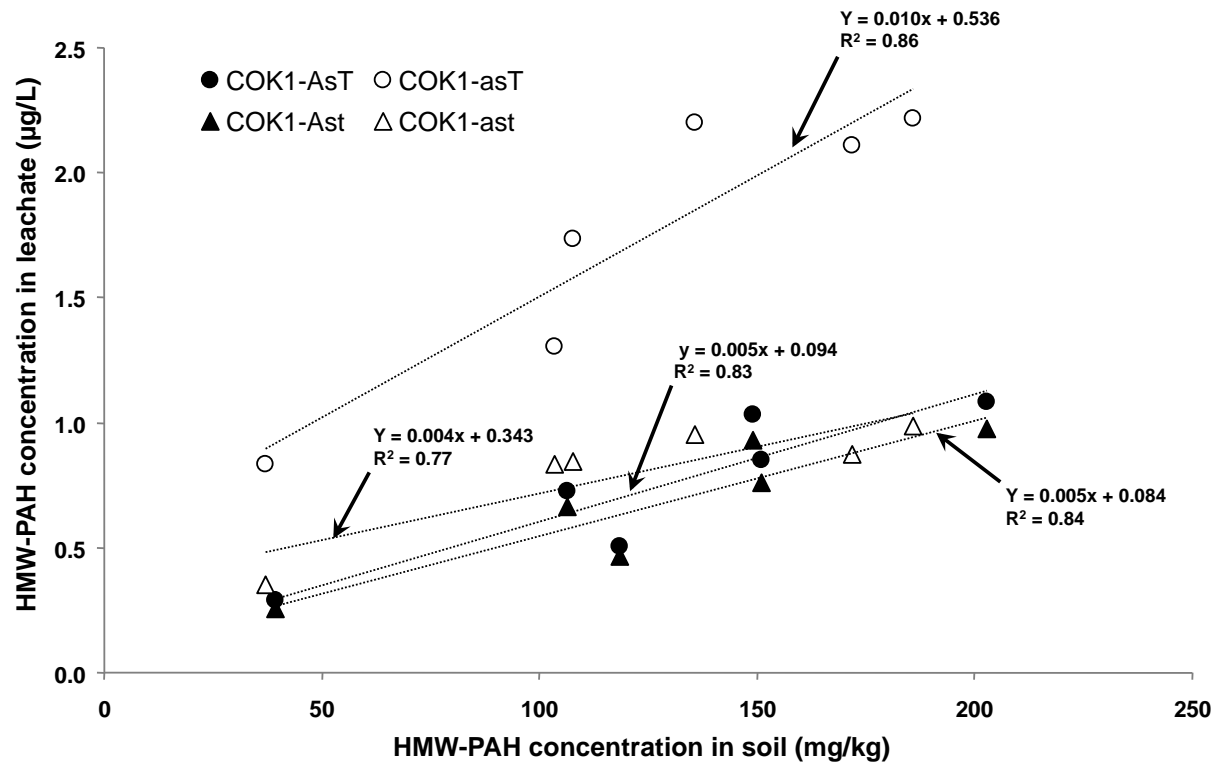


Figure S2: High molecular weight (HMW) PAH concentrations in the leachates ($\mu\text{g/L}$) for AsT (●), Ast (▲), asT (○) and ast (△) conditions as a function of the HMW-PAH concentration in the COK1 soil (mg/kg). Upper and lower cases correspond to high and low parameter levels respectively.

HMW-PAHs: Sum of high molecular weight (low solubility) PAH concentrations (benzo(a)anthracene to benzo(ghi)perylene).

Table S1: Batch leaching test conditions of temperature (T and t), ionic strength (S and s) (Electrical Conductivity) and availability (A and a) levels used for the design of experiments with COK1 and COK2 soils (upper and lower cases correspond to high and low parameter levels, respectively) and pH value, DOC, Σ 15 PAH, Σ 11 O-PAC and Σ 5 N-PAC concentrations of the leachates.

15 PAHs: Σ 16 US EPA PAHs except naphthalene. LMW-PAHs: Sum of low molecular weight PAH concentrations (acenaphthylene to pyrene). HMW-PAHs: Sum of high molecular weight PAH concentrations (benzo(a)anthracene to benzo(ghi)perylene). Σ 11 O-PACs: Sum of the 11 quantified O-PAC concentrations. Σ 5 N-PACs: Sum of the 5 quantified N-PAC concentrations. RSD: Relative Standard Deviations calculated from the results of the triplicates.

DOE	T (°C)	EC (µS/cm)	A (%)	pH	DOC (mg/L)	Σ 15 PAHs (µg/L)	LMW-PAHs (µg/L)	HMW-PAHs (µg/L)	Σ 11 OPACs (µg/L)	Σ 5 NPACs (µg/L)
COK1-AST	28	5740	100	8.0	32.2	180.3	176.4	3.9	222.1	73.2
COK1-aST	28	5580	0	8.0	10.7	59.9	57.4	2.5	72.0	14.6
COK1-AsT	28	556	100	8.6	37.0	185.3	175.9	9.4	208.5	72.5
COK1-asT	28	532	0	8.8	14.4	77.9	61.7	16.2	69.8	14.2
COK1-ASt	3	5544	100	8.5	24.8	156.4	153.0	3.4	183.8	60.8
COK1-aSt	3	5550	0	8.6	7.2	49.0	47.0	2.0	64.3	11.8
COK1-Ast	3	496	100	9.3	29.7	169.5	161.3	8.2	181.9	60.6
COK1-ast	3	487	0	9.2	10.7	66.8	58.2	8.6	71.8	12.2
RDS (%)	0	1	0	0	2	8	9	4	12	1
COK2-AST	28	5960	100	7.6	50.1	156.9	154.9	2.0	165.3	55.2
COK2-aST	28	5800	0	7.4	17.0	38.3	37.4	0.9	34.8	8.6
COK2-AsT	28	2105	100	7.7	50.8	188.2	186.0	2.2	192.0	64.0
COK2-asT	28	2042	0	7.8	19.2	36.4	35.4	1.0	31.8	7.8
COK2-Ast	3	5635	100	8.4	37.2	124.4	122.8	1.6	124.3	46.9
COK2-aSt	3	5680	0	8.2	12.2	28.7	28.4	0.3	25.3	4.9
COK2-Ast	3	2039	100	8.3	39.0	139.0	137.5	1.5	139.6	43.6
COK2-ast	3	1995	0	8.2	13.2	29.9	29.4	0.5	25.5	5.5
RDS (%)	0	1	0	1	4	4	4	10	7	4

Table S2: Batch leaching test conditions used for the design of experiments with COK1 and COK2 soils for triplicate lixiviated under intermediate conditions: Temperature (T), ionic strength (Electrical Conductivity, EC), availability (A], pH. Characteristics of the obtained leachates: DOC, Σ 15 PAH, Σ 11 O-PAC and Σ 5 N-PAC concentrations.

15 PAHs: Σ 16 US EPA PAHs except naphthalene. LMW-PAHs: Sum of low molecular weight PAH concentrations (acenaphthylene to pyrene). HMW-PAHs: Sum of high molecular weight PAH concentrations (benzo(a)anthracene to benzo(ghi)perylene). Σ 11 O-PACs: Sum of the 11 quantified O-PAC concentrations. Σ 5 N-PACs: Sum of the 5 quantified N-PAC concentrations. RSD: Relative Standard Deviations calculated from the results of the triplicates.

DOE	T (°C)	EC (µS/cm)	A (%)	pH	DOC (mg/L)	Σ 15 PAHs (µg/L)	LMW-PAHs (µg/L)	HMW-PAHs (µg/L)	Σ 11 OPACs (µg/L)	Σ 5 NPACs (µg/L)
COK1-R1	16	3035	50	8.5	18.5	161.8	157.4	4.4	183.3	45.0
COK1-R2	16	3052	50	8.5	18.3	178.7	174.1	4.7	211.4	44.9
COK1-R3	16	3015	50	8.5	17.9	155.1	150.5	4.5	173.2	44.3
RDS (%)	0	1	0	0	2	8	9	4	12	1
COK2-R1	16	3700	50	8.1	29.0	97.6	95.8	1.8	85.2	23.3
COK2-R2	16	3657	50	8.0	27.2	104.5	102.6	1.9	95.5	24.9
COK2-R3	16	3688	50	8.1	27.1	103.0	101.4	1.6	92.8	24.7
RDS (%)	0	1	0	1	4	4	4	10	7	4

Table S3: Ions monitored by GC-MS in single ion monitoring (SIM) mode for the 16 US-EPA PAHs, 11 O-PACs and 5-N-PACs with their associated internal standards (IS) for extraction and quantification

Quantification IS	m/z	Extraction IS	m/z	PAH	m/z
Naphtalene-D8	136	Dibenzofurn-D8	176	Naphtalene	128
Acenaphtylene-D10	164	Fluorene-D10	176	Acenaphtylene	152
				Acenaphthene	153
				Fluorene	166
Phenanthrene	178				
Phenanthrene-D10	188	Anthracene-D10	188	Anthracene	178
Pyrene-D10	212	Fluoranthene-D10	212	Fluoranthene	202
				Pyrene	202
Chrysene-D12	240			Benz[a]anthracene	228
				Chrysene	228
				Benzo[b]fluoranthene	252
				Benzo[k]fluoranthene	252
Perylene-D12	264			Benzo(ghi)perylene-D12	276
		Indeno[1,2,3-c,d]pyrene	276		
		Dibenzo(ah)anthracene	278		
		Benzo[ghi]perylene	276		

Quantification IS	m/z	Extraction IS	m/z	PAH	m/z
Acenaphtylene-D10	164	Dibenzofurn-D8	176	Dibenzofuran	168
9H-Fluorenone-D8	188	Anthraquinone-D8	216	9H-fluorenone	180
				Perinaphtenone	152
				Anthraquinone	208
				Cyclopenta(def)phenanthrone	204
Pyrene-D10	212	Fluoranthene-D10	212	Methylanthracene-9,10-dione	165
				Benzo(a)fluorenone	230
Chrysene-D12	240			Benzanthrone	230
				Benzoanthracenedione	258
				Naphtacene-5,12-dione	258
				Benzo(cd)pyrenone	254

Quantification IS	m/z	Extraction IS	m/z	PAH	m/z
Quinoline-D7	136	Dibenzofurn-D8	176	Quinoline	129
9H-Fluorenone-D8	188	Anthraquinone-D8	216	Benzo(h)quinoline	179
				Acridine	179
				Carbazole	167
Pyrene-D10	212			Benzo(c)acridine	229

Table S4: Soil specific area (m²/g), Extractable Organic Matter (EOM) contents (g/kg), coal-tar molecular weight (MW_{ct} – g/mol), 16 US-EPA PAH, 11 O-PAC and 5 N-PAC concentrations of COK1 and COK2 soils, before and after the thermal treatment (100°C during 5 days under argon atmosphere). RSD: relative standard deviation

	Subcooled Solubility (mg/L)	COK1 soil			COK2 soil		
		Initial	Preheated	% RSD	Initial	Preheated	% RSD
Specific area (m²/g)		12.8	5.9	7	15.1	11;4	4
EOM (g/kg)		21.4	21.6	4	14;3	15;2	6
MW_{ct} (g/mol)		211	256	8	338	386	13
PAHs (mg/kg)							
Naphtalene	99,4916	31	30	8	20	26	13
Acenaphtylene	19,4139	95	60	15	38	28	20
Acenaphthene	19,1608	14	10	22	32	22	11
Fluorene	10,4878	27	17	11	33	18	24
Phenanthrene	4,0830	128	135	10	111	109	13
Anthracene	3,8105	113	92	19	55	35	23
Fluoranthene	1,0137	488	502	15	173	174	10
Pyrene	0,9034	374	387	15	117	114	10
Benz[a]anthracene	0,1408	217	228	9	73	72	10
Chrysene	0,0930	197	239	10	64	74	10
Benzo[b]fluoranthene	0,0348	186	203	9	54	59	12
Benzo[k]fluoranthene	0,0348	104	106	8	32	33	11
Benzo[a]pyrene	0,0156	172	149	11	50	46	14
Indeno[1,2,3-c,d]pyrene	0,0551	136	151	9	41	46	12
Dibenzo[ah]anthracene	0,0168	37	40	10	11	12	11
Benzo[ghi]perylene	0,0167	108	119	10	32	36	12
Σ 16 PAHs (mg/kg)		2424	2470	11	936	904	10
O-PACs (mg/kg)							
Dibenzofuran	17,3970	30	30	19	29	30	7
9H-fluorenone	23,7550	27	43	12	21	33	10
Perinaphtenone	-	6	6	9	4	3	20
Anthraquinone	38,7705	17	21	8	11	14	9
Cyclopenta[def]phenanthrone	8,3195	36	46	10	14	18	6
Methylantracene-9.10-dione	14,6833	8	11	10	4	7	13
Benzo[a]fluorenone	0,7116	72	118	8	25	41	9
Benzanthrone	0,7625	55	65	10	13	16	11
Benzoanthracenedione	1,2650	13	23	9	6	9	13
Naphtacene-5.12-dione	1,2650	20	25	8	4	5	18
Benzo[cd]pyrenone	-	48	54	6	16	19	18
Σ 11 O-PACs (mg/kg)		333	442	8	148	196	7
N-PACs (mg/kg)							
Quinoline	6110,0000	1	1	22	1	1	11
Benzo[h]quinoline	78,2324	1	1	15	1	1	7
Acridine	38,3166	2	1	25	1	1	12
Carbazole	1,7917	11	11	19	7	6	10
Benzo[c]acridine	-	17	19	3	8	8	9
Σ 5 N-PACs (mg/kg)		31	32	7	18	18	8
Total PACs (mg/kg)		2787	2944		1102	1117	