Time-dependent multivariate and spectroscopic characterization of oil residue in Niger Delta soil

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Supporting information

Table S1 Structural spectrometric indices obtained from Infrared region (Permanyer et al.,)[1]

Structures indices	Formulae
Aromatic index	$A_{1600}/\sum A$
Aliphatic index	$A_{1600} + A_{1376}/\sum A$
Branched index	$A_{1376}/A_{1460} + A_{1376}$
Long-chain index	$A_{724}/A_{1460} + A_{1376}$(Aliphatic structures)
Carbonyl index	$A_{1700}/\sum A$
Sulfoxide index	$A_{1030}/\sum A$(Oxygenated function)
$\sum A$	$A_{1700} + A_{1600} + A_{1460} + A_{1376} + A_{1030} + A_{846} + A_{814} + A_{743} + A_{724} +$

* The subscripts represent the wavenumbers under which the areas were obtained, $\sum A =$ The sum of areas identified in the spectrum.

Table S2. UV absorption maxima and absorption ratios for oil residues

Samples	Age of spill (yrs)	λ_1 (nm)	λ_2 (nm)	A_{205}/A_{215}	A_{228}/A_{256}	A_{248}/A_{267}	A_{248}/A_{278}
S1	10	228	278	1.413	1.477	0.817	0.849
S2	10	228	274	1.440	1.364	0.747	0.751
S3	8	226	264	1.418	1.466	0.975	1.084
S4	5	226	258	1.483	1.477	0.983	1.094
S5	2	226	272	1.525	1.234	0.798	0.802
S6	1	228	262	1.213	1.532	0.823	0.875
B1	1	230	254	1.485	1.898	1.204	1.481
B2	1	230	258	1.485	1.514	0.979	1.092
FC	NA	224	256	1.434	2.946	1.000	1.281

Table S3. Assignment of IR absorption bands.

Wavelength (cm^{-1})	Assignment
3425	ν (N-H), H-bond pyrrollic group
3400	ν (O-H), inter H-bonded, broad band
3040	$\nu(C\text{-}H)_{ar}$, aromatic or unsaturated
2920,2850	ν (C-H), of aliphatic CH_2 and CH_3
1775	ν (C=O), ester with electron-withdrawing group attached to single-bonded oxygen, like Ar-C-O-R
1735*	ν (C=O), ester
1720-1690*	ν(C=O), ketone, aldehyde, carboxylic
1650-1630*	N(C=O), highly conjugated ketone Ar-CO-R
1600	ν (C=C), aromatic
1590-1560	$\nu(COO^-$ carboxylic salt)
1490*	Aromatic ring stretch frequency
1450	$\delta(CH_2 + CH_3)$, bending vibrations
1375	$\delta(CH_3)$, bending vibrations
1300-1100*	ν(C-O) and ν(O-H), in phenoxyl structure, ethers and vibrations of –S-linkages
1100-1000	ν(C-O), aliphatic ether, alcohol
1030	(S=O) Sulphoxide
875	$\gamma(CH_{ar1})$, isolated aromatic H
810-5	$\gamma(CH_{ar2,3})$, isolated two and/or three H on aromatic ring
750	$\gamma(CH_{ar4})$, 1,2 substituted, 4 neighbouring H
784*	$r(CH_2)_{n,\ n<4}$, alkyl chain
720	$r(CH_2)_{n,\ n>4}$, alkyl chain

*Very weak shoulder band to nearby broad base band

Table S4 Spectrometric index calculated from IR region

	Aromatic Index	Aliphatic Index	Branched Index	Long chain Index	Carbonyl Index	Sulfoxide Index	$\sum A$
S1	0.04	0.04	0.82	2.66	0.02	0.06	57.99
S2	0.01	0.05	0.89	3.19	0.01	0.06	55.20
S3	0.02	0.05	0.88	2.59	0.01	0.06	56.89
S4	0.01	0.05	0.88	2.89	0.00	0.06	55.83
S5	0.02	0.05	0.91	2.58	0.03	0.06	58.43
S6	0.02	0.04	0.79	2.37	0.02	0.06	56.85
B1	0.01	0.05	0.88	3.00	0.02	0.01	48.38
B2	0.01	0.06	0.88	3.69	0.03	0.01	48.75
FC	0.04	0.04	0.82	2.98	0.00	0.06	53.36

Table S5 Gas chromatography weathering index

Sample*	Time of spill (years)	Pr/Ph	Pr/ n-C_{17}	Ph/ n-C_{18}	CPI	(Pr +n-C_{17})/ (Ph + n-C_{18})
S1F1	10	1.190	5.512	4.312	1.029	0.061
S2F1	10	0.740	5.814	6.763	1.029	0.532
S3F1	8	0.790	3.421	6.614	1.035	0.062
S4F1	5	1.220	6.601	4.971	1.034	0.871
S5F1	2	1.151	3.082	3.774	1.034	0.772
S6F1	1	1.561	2.711	2.463	1.042	0.894
FCF1	NA	1.192	2.362	1.725	1.050	1.073

$$CPI = \frac{\sum (nC_{11} to\ nC_{27})}{\sum (nC_{10} to\ nC_{26})}$$

* F1 means saturate fraction of samples,

References

1 A. Permanyer, L. Douifi, A. Lahcini, J. Lamontagne and J. Kister, *Fuel,* 2002, **81**, 861-866.