SUPPORTING INFORMATION

Assimilation and Transport of Organic Bound Tritium in an Irrigated Pine Forest

M.C. Duff*, W.W. Kuhne, B. Viner, A. Swindle, A. Houk, S. Chiswell, D.B. Hunter and O.E. Rivera.

Savannah River National Laboratory (SRNL), Savannah River Site (SRS), Aiken, SC 29808. *Corresponding Author: Martine C. Duff, Ph: 803-725-2054; E-mail: <u>Martine.Duff@srnl.doe.gov</u> **Fig. S1.** The MWMF forest lies true north of the holding pond, which is used for the irrigation of the MWMF forest trees—Adapted from SRNS (2014).¹



Table S1.	Typical contaminant	and water quality values fo	or MWMF irrigation pond water.*
-----------	---------------------	-----------------------------	---------------------------------

Component	Method	Range	Units	Comments
1,2-dichloroethylene	EPA8260B	0.29 to 20	μg L ⁻¹	Most of these

1,4-dioxane		3.7 to 20		
Acetone]	2.3 to 9.21]	compounds are DCDA
cis-1,2-dichloroethylene		2.5 to 20		and CEPCI A listed
Tetrachloroethylene		0.057 to 1.1		and CERCLA listed.
Trichloroethylene		0.89 to 10.0		
Ethylene		0.048 to 0.12		
Methane	AIVIZUGAA	<u><</u> 1,300	μgι	
Nitrate	EPA9056 & 300.0	0.30 to 0.38	mg 1-1	
Nitrate-nitrite as N	EPA353.1	0.08 to 0.31	IIIg L	
Redox potential (E _h)		+84 to +305	mV	
рН		4.6 to 9.5		Average: 6 to 6.5
Specific conductance		27 to 348	µS cm⁻¹	Average: 30 to 40
Total CaCO ₃ alkalinity		0 to 80		Average: 3 to 9
Total dissolved solids	EPA160.1	46 to 50	mg L ⁻¹	
Total organic carbon	EPA9060	9.4 to 10.0		
Total organic halogens	EPA9020B	0.023 to 0.042	μg L ⁻¹	
Turbidity		0.9 to 48.8	NTU	
Temperature		4.3 to 34.8	°C	
Aluminum	EPA6010B	36.4 to 37.8		
Barium	EPA6020A	36.8 to 110		
Calcium	EPA6010B & 6020A	1,900 to 2,330		
Cobalt	EPA6010B, 6020A & B	2.00 to 2.04		
Copper	EPA6020A & B	<u>≤</u> 1.39		
Iron	EPA6010B & 6020A	2,520 to 6,380	ug 1-1	
Magnesium		1,270 to 1,600	μgι	
Manganese	LFA0010B	29.8 to 323		
Nickel	EPA6010B, 6020A & B	0.854 to 1.86		
Potassium		971 to 1,620		
Selenium		3.5 to 5.0		
Strontium	EPA6020A	<u>≤</u> 12.1		
¹⁴ C	LSC	Up to 40.7		
Gross alpha	Alpha counting	Up to 0.15		
¹²⁹	LSC	0.02 to 0.31	Dal-1	
Non-volatile beta	LSC	0.01 to.0.73	BY L-	
Total radium	EPA903.0MOD	0.04 to 0.09		
⁹⁹ Tc	Radiometric counting	Up to 1.89		
Tritium	LSC	5,923 to 574,074		Average: ~54,000,000

*Data provided by the SRS ACP as part of their 2012 to 2017 monitoring studies. NTU: Nephelonic Turbidity Units.

¹ Savannah River Nuclear Solutions (SRNS), Mixed Waste Management Facility Groundwater Remediation. Fact Sheet. Updated on 09/22/2014, Aiken, SC 2014.

Table S2. Analysis protocols for various biological sample matrices. HTO, E-OBT and NE-OBT were extracted sequentially whereas total tritium was isolated in by complete sample combustion. Total OBT extraction (E-OBT plus NE-OBT) from water occurred via the NE-OBT step (only) on Whatman #10 filtrate.

Matrix	нто	E-OBT	NE-OBT	Total Tritium from Complete Combustion		
Bark,			Heat to 300°C at a ramp rate			
litter		Rinse at room temp. with tritium- free water for 72 b	600°C at 7°C min ⁻¹ ; continue to 600°C at 7°C min ⁻¹ and hold 60 min collect tritium in 10 mL 0.1 M nitric acid (HNO ₃) in bubbler trap. Heat to 600°C at 5°C min ⁻¹	Heat to 155°C at a ramp rate of		
				3.5°C min ⁻¹ and hold for 12 min at		
	Heat to			air flow of 0.2 L min ⁻¹ ; Heat to 600°C at 5°C min ⁻¹ at oxygen (O ₂) flow of 0.2 L min ⁻¹ to facilitate combustion and hold for 20 min collected in 10		
Tree	150°C at					
cores	rate of		with	with	and hold 60 min collect	mL 0.1 M HNO _{3} in bubbler trap.
	2.5°C		tritium in 10 mL 0.1 M HNO ₃	5 1		
Soil	min ⁻¹ and		Heat to 300°C at 5°C min ⁻¹ :	Heat to 155°C at 3.5°C min ⁻¹ and		
	hold for		water	continue to 600°C at 7°C	hold for 12 min at air flow of 0.2 L	
	50 11111.	101 72 11.	min ⁻¹ and hold 20 min;	min ⁻¹ ; Heat to 600°C at 5°C min ⁻¹ at		
			continue to 900°C at 10°C	O_2 flow of 0.2 L min ⁻¹ and hold for 30		
			min ⁻¹ and hold 15 min;	min; Heat to 900°C at 8°C min ⁻¹ with		
			M HNO ₂ in bubbler trap.	HNO_2 in bubbler trap.		
Matrix			Total ¹⁴ C as CO ₂ by Comple	te Combustion		
Any	A second bubbler trap was used after tritium collection for $^{14}CO_2$ capture. The					
	liberated ¹⁴ CO ₂ is trapped in Carbo Sorb E scintillation cocktail, which was counted					

Wavelength	Band Assignment	Band Origin
(cm⁻¹)		
805	Glucomannan ^A ; vibration (vibr) of mannan in hemicellulose (hemiC), and C-H	Polysacchar-
	out-of-plane bending in phenyl rings ^B	ide (polyS) ^{A,B}
825	C-H out-of-plane bending in guaiacyl units ^B	Lignin (lgn) ^B
853-860	C-H out-of-plane in position 2, 5 and 6 of guaiacyl units ^{A,B}	lgn ^{A,B}
892-900	Aromatic (arom) C-H out-of-plane deformation (deform) ^c ; anomeric C-	cel/hemiC/pe
	groups, C ₁ -H deform, ring valence vibr ^c ; C-H deform of beta-glycosidic	ctin ^c , polyS ^{A,B}
	linkages in cellulose (cel) ^B ; anti-symmetric out-of-phase stretching (strh) in	
	pyranose ring ^D ; C_1 vibr ^E	
945	O-H out-of-plane deform in carboxylic acid (R–COOH) ^B	Terpenoids ^B
960	C-H out-of-plane deform in Ign ^B	lgn [₿]
985	C-O strh in cel ^B	polyS [₿]
998-1005	C-O strh in cel ^{A,B} and hemiC ^A	polyS ^{A,B}
1024-1035	C-O strh ^c ; C-O deform in primary alcohols (R-OH), unconjugated (unconj.)	hemiC ^{A,C,E} ,
	C=O strh, arom C-H in-plane deform in lgn, C-O and C-C strh and CH ₂ rocking	cel ^{A,C} , lgn ^{A,B,E}
	in cel ^A ; C-O strh in primary R-OH in cel ^B ; C-O-C deform ^D ; C-O strh vibr ^E	polyS ^{A,B} ,
1055-1060	C-O strh vibr of cel and hemiC ^A ; C-O strh of secondary ROH ^B ; C-O strh vibr ^E	polyS ^{A,B} ,
		cel/hemiC ^E
1101-1106	Ring asymmetric (asym) valence vibr ^c ; C-O and C-C strh and CH ₂ rocking in	polyS ^{A-C}
	cel ^A ; C-O-C strh in cel and hemiC ^B	
1128	Syringyl Ign and C-O, C-H deform in syringyl Ign, C-O strh ^D	
1140	Guaiacyl Ign and C-O, C-H deform in guaiacyl Ign, C-O strh ^D	
1155-1160	C-O-C symmetric (sym) strh ^c ; C-O-C asym strh vibr in cel and hemiC ^{A,B} ; C-O-C	cel/hemiC ^c ,
	asym strh in cel I and II ^E	polyS ^{A,B}
1185	C-O strh in cel ^B	polyS ^B
1200-1205	O-H in-plane bending in cel I and II ^A	polyS ^A
1221-1230	Syringyl ring and C-O strh ^c ; C-C, C-O, and C=O strh, acetyl and carboxylic vibr	lgn ^{A,C} , xylan ^C ,
	in xylan ^A ; O-H vibr in guaiacyl ring, C-C, C-O and C=O strh in lgn ^B	polyS ^A
1264-1270	Guaiacyl ring plus C=O strh ^{A,C} ; acetyl and carboxylic vibr in xylan ^A ; C-O vibr in	Guaiacyl-Ign ^c ,
	guaiacyl rings ^B ; syringyl ring breathing and C-O strh in Ign and xylan ^E	polyS ^A , Ign ^{A,B}
1315-1317	CH ₂ rocking vibr ^c ; CH ₂ wagging in crystalline cel ^B	cel ^c , polyS ^B
1320-1330	Phenolic O-H, syringyl and guaiacyl (ring) condensed, C=H vibr in polyS ^A ; C-H	lgn/polyS ^A
	of methyl (Me) groups in methoxy of amorphous cel ^B ; C ₁ -O vibr in syringyl	
	derivatives, C-H in-plane bend in cel I and II ^E	
1360-1372	C-H deform vibr ^c ; phenolic O-H, aliphatic C-H strh in CH ₃ , not in O-Me, C-H	cel ^c , lgn ^A ,
	vibr in polyS ^A ; C-H deform in cel and hemiC ^B ; aliphatic C-H strh in Me and	polyS ^{A,C}
	phenolic OH ^E	
1385	C-O strh in cel and hemiC ^B	
1405	C=O in carboxylic groups in R–COOH and esters ^B	Terpenoids ^B
1420-1430	Arom skeletal (skl) vibr with C-H in-plane deform in Ign and polyS ^A ; C-H asym	lgn ^{A,B} , polyS ^A
	deform in methoxyl, arom skl vibr, Ign ^B ; arom ring and CH, benzene (benz)	
	skl with C-H deform ^D and strh ^E	
1450-1453	C=C and C-H bond, O-H in-plane deform ^c	lgn, hemiC ^c

Table S3. FTIR assignments made for tree core material based on peak matching with reference databases and literature.

1460-1470	C-H deform, asym in -CH ₃ and -CH ₂ - ^A ; C-H asym deform in methoxyl for lgn,	lgn ^{A,B} , polyS ^A
	asym in -CH ₃ and CH ₂ in pyran for hemiC ^B ; C-H deform ^D ; CH ₂ deform strh in	
	Ign and xylan ^E	
1500-1515	C=C strh of arom skl vibr ^C ; arom skl vibr ^{A,E} ; C=C strh of arom ring, C=O bond	lgn ^{A-C}
	vibr in extractants ^B ; arom/benz ring strch vibr ^D	
1590	Skl vibrations from the C-C ^B	lgn ^B
1593-1610	Arom skl and C=O strh vibr ^{A,C} ; C=O strh conjugated (conj) to arom ring and	lgn ^{A,C}
	carboxylic groups of Ign, R–COOH, esters ^B ; arom/benz ring strh vibr ^D	
1635	Absorbed O-H and conj C-O in polyS ^B	
1640	C=O strh vibr in conj carbonyl of Ign ^E	
1655-1675	C=O strh on conj <i>p</i> -subst aryl ketones ^A ; absorbed O-H and conj C-O in polyS ^B	lgn ^A
1690	C=O vibr in carboxylic group in resin acid ^B	Terpenoids ^B
1709-1750	C=O strh of acetyl and carbonyl groups ^c ; C=O strh in unconj ketones and	hemiC ^c , Ign ^A ,
	ester groups (usually polyS origin), conj aldehydes and R–COOH absorb	polyS ^{A,B}
	\leq 1700 cm ^{-1 A} ; C=O carbonyls in ester and acetyl groups in xylan ^B ; in	
	aldehydes and acids, unconj C=O and ketone strh ^{D,E}	
2850-2970	C-H strh, CH_2 , CH , and CH_3^D	
3400	O-H strh, O-H of R-OH, phenols, and acids ^D	

A. M. Traoré, J. Kaal and A.M. Cortizas, Differentiation between pine woods according to species and growing location using FTIR-ATR, *Wood Sci Technol.* Springer Publ. 2017.

- B. E. Gifty, G.E. Acquah, B.K. Via, O.O. Fasina and L.G. Eckhardt, Rapid quantitative analysis of forest biomass using Fourier transform infrared spectroscopy and partial least squares regression, *J. Analyt. Meth. Chem.* 2016, 1839598.
- C. O. Özgenç, S. Durmaz, and S. Kuştaş, Chemical analysis of tree barks using ATR-FTIR spectroscopy and conventional techniques, *BioResour*. 2017, **12**, 9143-9151.
- D. H. Bouafif, Ph.D. Thesis, L'Institut des Sciences et Industries du Vivant et de l'Environnement (Agro Paris Tech) est un Grand Etablissement dépendant du Ministère de l'Agriculture et de la Pêche, composé de l'INA PG, de l'ENGREF et de l'ENSIA. Quebec, Canada, 2010.
- E. S.J. Chapman, C.D. Campbell, A.R. Fraser, and G. Puri, FTIR spectroscopy of peat in and bordering Scots pine woodland: relationship with chemical and biological properties, *Soil Biol. Biochem.* 2001, **33**, 1193-1200.