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Supporting Information for The behaviour of low molecular weight organic carbon-14 containing compounds in contaminated groundwater during denitrification and iron-reduction.

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This consists of five sections, S1, S2, S3, S4 and S5.

S1. Method for ¹⁴C measurement in solid fraction

In to a 250 mL reaction vessel 1 ±0.01g of sediment was added with a magnetic stirrer. The system was sparged with N₂(g) prior to and during the extraction process, gas flow rate was set to 40 mL/min. Once sparged the reaction vessel was attached to two 125 mL gas washing bottles, the first of which contained 100 mL of Carbo-Sorb E and the second 100 mL of 1 M NaOH (acting as a safety bottle to ensure no release of $^{14}CO_2(g)$). 20 mL of 2 M H₂SO₄ was added to the reaction vessel to achieve a pH ~ 3 when buffered by sediment. It was left to react for 30 minutes before disconnecting the gas washing bottles and exchanging for duplicate wash bottles. For the oxidation step 20 mL of 5% potassium persulfate and 4 mL 4% AgNO₃ were added to the container and heated to 80-90 °C. Further additions of K₂S₂O₈ and AgNO₃ at the same concentration and volume were made after one and two hours of reaction. The system was left for another hour to give a total oxidation reaction time of 3 hours. Triplicate samples of 1 mL were collected from wash bottles containing Carbo-Sorb E and mixed with 10 mL of PermaFluor E (Ahn et al., 2003; Magnusson et al., 2007). All samples were left to dark adjust for 24 hours prior to counting on the liquid scintillation counter.

S2. Experimental results for complete run

Experiments were run until a minimum of 80% of any ¹⁴C-labelled LMWO was removed from solution. The complete data sets from addition of LMWO to the completion of the experiments for each condition are shown below.

S2.1 Nitrate amended microcosms, 7 to 22 days.



Figure S1 The results of the complete run of denitrification experiments (7 to 22 days) a) the percentage of ¹⁴C in solution; b) pH; c) concentration of nitrite in solution; d) concentration of nitrate in solution (original nitrate addition = 10 mM, t=7 indicates time of ¹⁴C addition). Error bars denote one standard deviation of triplicate measurements; where not shown error bars are less than the size of the symbol used.



Figure S2 The results of the complete run of iron-reducing experiments (28 to 60 days) a) the percentage of 14 C in solution; b) pH; c) fraction of Fe(II) in solids; d) concentration of Fe $^{2+}$ in solution. Error bars denote one standard deviation of triplicate measurements; where not shown error bars are less than the size of the symbol used.

S3. Results of control experiments

Control experiments were run concurrently with active microcosms with the same incubation time to establish the desired redox condition. After the incubation time (7 days and 28 days for denitrification and iron reduction respectively) the microcosms were autoclaved at 120° for 30 minutes to eliminate microbial activity and the LMWO was added. The experiments were then run over the subsequent seven days to determine any abiotic processes which may affect the aqueous ¹⁴C concentration of the LMWO. The results of these experiments are shown below.

S3.1 Nitrate amended control microcosms



Figure S3 The results of the denitrification control experiments a) the percentage of 14 C in solution; b) pH; c) concentration of nitrite in solution; d) concentration of nitrate in solution (original nitrate addition = 10 mM, t=7 indicates time of LMWO addition). Experiment duration from day 7 to day 14.



Figure S4 The results of the iron-reducing control experiments a) the percentage of ${}^{14}C$ in solution; b) pH; c) fraction of Fe(II) in solids; d) concentration of Fe²⁺ in solution. Experiment duration from day 28 to day 35.

S4. OTU table

Table S1 Summary OTU table with all identified phylum and significant orders (italics) for all samples

	Unaltered				fication	Iron-reducing					
	А	В	С	Acetate	Formate	Formaldehyde	Methanol	Acetate	Formate	Formaldehyde	Methanol
Acidobacteria	28.30	29.99	26.01	34.88	35.45	28.08	7.69	24.69	24.29	10.60	19.23
Actinobacteria	14.54	6.48	10.10	9.56	9.07	14.66	6.63	11.93	14.34	9.11	3.79
Armatimonadetes	1.23	1.06	2.03	1.01	1.00	0.86	0.09	0.23	0.28	0.45	2.28
Bacteroidetes	1.02	2.43	5.76	1.55	1.58	5.50	5.38	3.81	3.36	4.27	3.91
Chlamydiae	0.01	0.01	0.26	0.01	0.02	0.17	0.01	0.01	0.02	0.01	0.04
Chloroflexi	1.14	1.08	1.69	2.04	1.39	1.95	0.91	2.19	2.06	0.56	1.90
Deinococcus-Thermus	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Gemmatimonadetes	2.61	0.89	2.16	2.92	3.26	2.07	0.77	2.01	2.29	1.72	2.66
Planctomycetes	7.37	10.48	10.80	7.95	7.94	5.75	2.87	6.79	7.52	4.85	5.23
Alphaproteobacteria	9.99	12.64	12.78	10.98	11.05	9.92	6.22	13.16	11.78	13.88	9.40
Betaproteobacteria	5.67	9.16	6.76	11.52	13.10	12.19	34.77	21.51	21.60	37.62	28.58
Burkholderiales	1.47	1.72	2.29	6.44	7.33	8.15	32.16	14.60	10.64	34.41	9.48
Methylophilales	0.00	0.01	0.12	0.00	0.00	0.18	0.01	0.00	0.00	0.11	0.11
Rhodocyclales	0.01	0.01	0.10	0.01	0.00	0.01	0.13	0.19	0.27	0.01	0.02
Deltaproteobacteria	1.51	2.08	2.32	0.90	0.94	1.16	0.22	0.69	0.52	0.63	1.06
Gammaproteobacteria	3.12	2.61	3.87	3.39	3.08	4.19	30.39	2.81	2.25	7.87	10.86
Chromatiales	0.02	0.01	0.09	0.12	0.08	0.07	0.01	0.06	0.02	0.02	0.05
Legionellales	0.05	0.07	0.24	0.03	0.07	0.19	0.02	0.04	0.03	0.12	0.19
Pseudomonadales	0.46	0.52	0.63	0.59	0.45	0.55	0.25	0.38	0.40	0.40	0.26
Xanthomonadales	0.23	0.62	1.15	0.39	0.42	1.69	29.69	0.77	0.62	5.75	4.42
Proteobacteria - unclassified	3.92	2.88	3.19	2.82	2.70	2.04	0.82	2.29	1.86	0.99	1.64
Spiro	0.01	0.03	0.02	0.01	0.01	0.00	0.00	0.00	0.00	0.00	0.00
Synergistetes	0.17	0.06	0.11	0.33	0.24	0.27	0.08	0.22	0.28	0.12	0.19
Verrucomicrobia	13.38	12.27	6.84	6.29	5.44	6.09	1.24	3.34	3.14	4.59	5.16
BRC1	0.05	0.12	0.08	0.02	0.02	0.02	0.00	0.00	0.00	0.07	0.01
candidate_division_WPS-1	0.37	0.50	0.55	0.24	0.25	0.39	0.07	0.10	0.10	0.18	0.35
candidate_division_WPS-2	0.34	0.64	0.63	0.44	0.33	0.49	0.08	0.20	0.21	0.22	0.31

Candidatus_Saccharibacteria	0.90	1.04	1.18	0.45	0.51	0.91	0.23	1.07	0.57	0.37	1.60
Cyanobacteria/Chloroplast	0.01	0.03	0.09	0.00	0.00	0.02	0.01	0.02	0.00	0.02	0.02
Firmicutes	2.02	0.92	1.64	2.03	1.89	1.35	1.22	2.40	2.99	0.64	0.85
Hydrogenedentes	0.01	0.02	0.02	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.01
Latescibacteria	1.64	2.33	0.75	0.32	0.30	1.76	0.16	0.13	0.18	1.15	0.75
Microgenomates	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Nitrospirae	0.65	0.25	0.27	0.34	0.43	0.16	0.15	0.38	0.35	0.05	0.17
Parcubacteria	0.01	0.00	0.08	0.00	0.00	0.01	0.00	0.00	0.00	0.02	0.02
Poribacteria	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
SR1	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

S5. Siderite precipitation

Solution composition	g/L in DIW
pН	6.7
Pe	0
KCl	0.006
MgSO ₄ .7H ₂ O	0.976
MgCl ₂ .6H ₂ O	0.081
NaCl	0.0094
Fe(II)	0.02
C as CO_3^{2-}	0.02

Tabla	C2 1-	mut	alution	aam	nonition	for	aidarita	nraai	nitation	modal
Table	52 H	ipuι	solution	com	position	101	siderne	preci	pitation	model

Geochemical modelling was undertaken using the PHREEQC (version 3) geochemical

speciation program (Parkhurst and Appelo, 2013) and the Hatches database (version

18)(Cross and Ewart, 1991). Siderite saturation index predicted to be +0.02 under these

conditions.

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