

## **Journal of Geophysical Research – Biogeosciences**

### **Supporting Information for:**

#### **Constraining the carbon budget of peat ecosystems: application of stoichiometry and enthalpy balances.**

Fred Worrall<sup>1</sup>, Ian. M. Boothroyd<sup>1</sup>, Gareth D. Clay<sup>2</sup>, Catherine S. Moody<sup>3</sup>, Katherine Heckman<sup>4</sup>, Tim P. Burt<sup>5</sup> and Rob Rose<sup>6</sup>

1. Department of Earth Sciences, Durham University, Science Laboratories, South Road, Durham, DH1 3LE, UK.
2. Department of Geography, School of Environment, Education and Development, University of Manchester, Oxford Road, M13 9PL, UK.
3. School of Geography, University of Leeds, Leeds, LS2 9JT, UK.
4. USDA Forest Service, Northern Research Station, Houghton, MI 49930, USA
5. Department of Geography, Durham University, Science Laboratories, South Road, Durham, DH1 3LE, UK.
6. Environmental Change Network, Centre for Ecology & Hydrology, University of Lancaster, Bailrigg, Lancaster, Cumbria, LA1 4YO, UK.

#### **Contents of this file**

S1 Table of Equations used within the study giving the Equation No. in the manuscript and the source when it is not this study.

S2. Table of compositional data used in this study.

S3. Table of radiocarbon ages used in this study.

**S1 Table of Equations used within the study giving the Equation No. in the manuscript and the source when it is not this study.**

Equation No.	Equation	Source
i	$6\text{CO}_2 + 6\text{H}_2\text{O} \xrightarrow{h\nu} \text{C}_6\text{H}_{12}\text{O}_6 + \text{O}_2$	
ii	$n\text{C}_6\text{H}_{12}\text{O}_6 + d\text{NH}_3 \rightarrow a\text{C}_{57}\text{H}_{86}\text{NO}_{35} + b\text{CO}_2 + c\text{H}_2\text{O}$	
iii	$\frac{[C]}{6} - \frac{r}{24} = GV$	McDermott and Loomis (1981)
iv	$C_{OX} = \frac{2[O]-[H]+3[M]}{[C]} = \frac{r}{[C]}$	Masiello et al. (2008)
v	$\frac{[C]_{pro}}{[C]_{sub}} - \frac{C_{ox}^{pro}[C]_{pro}}{(C_{ox}^{CO2}-C_{ox}^{sub})[C]_{sub}} = SEV$	
vi	$PV = E_gGV = E_gSEV$	Lafitte and Loomis (1988)
vii	$[C]_{CO2} = \frac{100}{[C]_{sub}} ([C]_{sub} - PV[C]_{pro})$	
viii	$100C_{pp} \Rightarrow 35C_R + 26C_{DOC} + 4C_{CH4} + 4C_{dissco2} + 9C_{POC} + 22C_{RES}$	Worrall et al. (2009)
xi	$\text{C}_6\text{H}_{12}\text{O}_6 + 0.08\text{NH}_4^+ \rightarrow 0.08\text{C}_{57}\text{H}_{86}\text{NO}_{35} + 1.44\text{CO}_2 + 0.78\text{H}_2\text{O} + 3.32\text{H}^+$	
x	$\text{C}_6\text{H}_{12}\text{O}_6 + 0.1\text{NH}_4^+ \rightarrow 0.1\text{C}_{49}\text{H}_{73}\text{NO}_{29} + 1.2\text{CO}_2 + 0.91\text{H}_2\text{O} + 4\text{H}^+$	
xi	$\text{C}_{57}\text{H}_{86}\text{NO}_{35} + 0.92\text{NO}_3^- + 4.63\text{O}_2 \rightarrow 1.92\text{C}_{25}\text{H}_{35}\text{NO}_{15} + 9.1\text{CO}_2 + 18.8\text{H}^+$	
xii	$\text{C}_{25}\text{H}_{35}\text{NO}_{15} + 3.65\text{O}_2 \rightarrow 0.53\text{C}_{39}\text{H}_{56}\text{NO}_{26} + 4.26\text{CO}_2 + 3.91\text{H}^+ + 0.47\text{NH}_4^+$	
xiii	$\text{C}_{39}\text{H}_{56}\text{NO}_{26} + 1.54\text{SO}_4 \rightarrow 0.43\text{C}_{75}\text{H}_{107}\text{NO}_{45} + 6.41\text{CO}_2 + 1.54\text{H}_2\text{S} + 4.75\text{H}^+ + 0.53\text{NH}_4^+$	

- xiv  $C_{39}H_{56}NO_{26} + 2.29NO_3^- \rightarrow 1.18C_{31}H_{38}NO_{24} + 2.27CO_2 + 2H^+ + 2.29NH_4^+$
- xv  $C_{39}H_{56}NO_{26} + 7.56H_2O \rightarrow 16.78CH_4 + 22.22CO_2 + NH_4^+$
- xvi  $\alpha C_{pp} - \beta C_{POC} = \chi C_{DOM} + \delta C_{CH_4} + \epsilon C_{RES} + \gamma C_{CO_2}$
- xvii  $C_{CO_2} = 0.07C_{DOM} + 3.54C_{CH_4} + 1.13C_{RES}$
- xviii  $C_{pp} - C_{POC} = 1.07C_{DOM} + 4.35C_{CH_4} + 2.13C_{RES}$
- xix  $1.07 = 2 - E_g SEV_{pp}^{DOM} \frac{[C]_{DOM}}{[C]_{pp}}$
- xx  $Depth = 0.047Age$
- xxi  $C_{sum} = 40 Age$
- xxii  $C_{39}H_{56}NO_{26} + C_{31}H_{38}NO_{24} \rightarrow 0.45C_{75}H_{107}NO_{45} + C_{29}H_{41}NO_{15} + 7CO_2$
-

**S2. Table of compositional data used in this study.**

<u>Name</u>	<u>Type</u>	<u>Detail</u>	<u>Month</u>	<u>Depth</u> <u>(cm)</u>	<u>Moles/100g</u>				
					<u>N</u>	<u>C</u>	<u>H</u>	<u>O</u>	<u>Cox</u>
Above Ground	Veg	Aboveground biomass			0.07	4.15	6.40	2.55	-0.26
Below Ground	Veg	Belowground biomass			0.09	4.23	6.30	2.48	-0.25
CHS	DOM	Streamwater DOM	December		0.10	2.81	3.47	2.33	0.53
CHS	DOM	Streamwater DOM	February		0.11	2.30	2.26	1.69	0.63
CHS BG Feb 14 b	DOM	Streamwater DOM	February		0.10	2.39	2.56	1.66	0.44
CHS BG Mar 14 b	DOM	Streamwater DOM	March		0.12	2.79	3.09	2.09	0.51
CHS BG May 14 b	DOM	Streamwater DOM	March		0.11	3.09	3.52	2.47	0.57
CHS BG Jun 14 b	DOM	Streamwater DOM	June		0.17	3.10	3.82	2.52	0.56
CHS BG Jul 14 b	DOM	Streamwater DOM	July		0.14	3.11	3.53	2.50	0.61
CHS BG Aug 14 b	DOM	Streamwater DOM	August		0.12	3.24	3.66	2.59	0.58
CHS BG Sep 14 b	DOM	Streamwater DOM	September		0.12	3.32	3.72	2.48	0.48
CHS BG Oct 14 b	DOM	Streamwater DOM	October		0.11	3.35	3.74	2.52	0.48
CHS BG Nov 14 b	DOM	Streamwater DOM	November		0.10	3.22	3.43	2.49	0.57
CHS BG Dec 14 b	DOM	Streamwater DOM	December		0.11	2.22	2.47	1.93	0.77
CHS BG Mar 15 b	DOM	Streamwater DOM	March		0.07	2.41	2.86	1.78	0.38
CHS BG Apr 15 b	DOM	Streamwater DOM	April		0.09	2.58	3.24	1.83	0.27

POM Jun 13	POM	Streamwater POM	June	0.17	3.18	5.23	1.98	-0.24
POM Sep 14	POM	Streamwater POM	September	0.32	3.60	6.02	1.95	-0.33
MH ERIO	Veg	Eriophorum		0.09	3.91	6.14	2.58	-0.18
Litter	Veg	Litter		0.17	4.17	5.96	2.48	-0.12
MH Litter	Veg	Litter		0.11	4.00	5.89	2.48	-0.16
MH C1 0-2	Peat	Peat soil core	0-2	0.13	4.06	5.70	2.38	-0.13
MH C1 2-4	Peat	Peat soil core	2-4	0.14	4.20	5.76	2.19	-0.23
MH C1 4-6	Peat	Peat soil core	4-6	0.13	4.20	5.88	2.16	-0.28
MH C1 6-8	Peat	Peat soil core	6-8	0.09	4.11	5.84	2.42	-0.18
MH C1 8-10	Peat	Peat soil core	8-10	0.09	3.95	5.86	2.48	-0.16
MH C1 10-12	Peat	Peat soil core	10-12	0.10	4.05	6.04	2.43	-0.22
MH C1 12-14	Peat	Peat soil core	12-14	0.12	4.07	6.00	2.38	-0.22
MH C1 14-16	Peat	Peat soil core	14-16	0.12	4.00	6.16	2.40	-0.25
MH C1 16-18	Peat	Peat soil core	16-18	0.15	4.06	6.25	2.29	-0.30
MH C1 18-20	Peat	Peat soil core	18-20	0.14	4.07	6.14	2.21	-0.32
MH C1 20-25	Peat	Peat soil core	20-25	0.13	4.17	6.26	2.40	-0.26
MH C1 25-30	Peat	Peat soil core	25-30	0.09	4.12	6.12	2.41	-0.25
MH C1 30-35	Peat	Peat soil core	30-35	0.09	4.19	6.03	2.37	-0.24
MH C1 35-40	Peat	Peat soil core	35-40	0.10	4.26	6.23	2.41	-0.26
MH C1 40-45	Peat	Peat soil core	40-45	0.10	4.25	6.19	2.25	-0.33
MH C1 45-50	Peat	Peat soil core	45-50	0.08	4.23	6.18	2.34	-0.30
MH C1 50-60	Peat	Peat soil core	50-60	0.07	4.35	6.10	2.35	-0.27
MH C1 60-70	Peat	Peat soil core	60-70	0.08	4.43	6.17	2.28	-0.31
MH C1 70-80	Peat	Peat soil core	70-80	0.09	4.33	6.26	2.30	-0.32
MH C1 80-90	Peat	Peat soil core	80-90	0.08	4.31	6.08	2.42	-0.23
MH C1 90-95	Peat	Peat soil core	90-95	0.08	4.26	6.04	2.46	-0.21
MH C1 95-100	Peat	Peat soil core	95-100	0.07	4.34	5.75	2.28	-0.23
MH C2 0-2	Peat	Peat soil core	0-2	0.10	4.12	6.02	2.35	-0.25
MH C2 2-4	Peat	Peat soil core	2-4	0.12	4.11	5.77	2.21	-0.24
MH C2 4-6	Peat	Peat soil core	4-6	0.13	4.18	5.73	2.16	-0.25
MH C2 6-8	Peat	Peat soil core	6-8	0.10	4.09	5.61	2.12	-0.27

MH C2 8-10	Peat	Peat soil core		8-10	0.07	3.90	5.84	2.56	-0.13
MH C2 10-12	Peat	Peat soil core		10-12	0.07	3.88	5.87	2.57	-0.14
MH C2 12-14	Peat	Peat soil core		12-14	0.07	3.91	5.85	2.42	-0.20
MH C2 14-16	Peat	Peat soil core		14-16	0.07	4.01	5.95	2.46	-0.20
MH C2 16-18	Peat	Peat soil core		16-18	0.07	3.90	5.70	2.61	-0.07
MH C2 18-20	Peat	Peat soil core		18-20	0.09	4.18	5.80	2.23	-0.25
MH C2 20-25	Peat	Peat soil core		20-25	0.10	4.26	5.77	2.20	-0.25
MH C2 25-30	Peat	Peat soil core		25-30	0.12	4.15	5.95	2.30	-0.24
MH C2 30-35	Peat	Peat soil core		30-35	0.10	4.21	5.87	2.34	-0.21
MH C2 35-40	Peat	Peat soil core		35-40	0.10	4.33	5.92	2.27	-0.26
MH C2 40-45	Peat	Peat soil core		40-45	0.09	4.24	5.97	2.32	-0.25
MH C2 45-50	Peat	Peat soil core		45-50	0.09	4.28	5.89	2.27	-0.26
MH C2 50-60	Peat	Peat soil core		50-60	0.08	4.36	5.89	2.30	-0.24
MH C2 60-70	Peat	Peat soil core		60-70	0.08	4.31	5.95	2.29	-0.26
MH C2 70-80	Peat	Peat soil core		70-80	0.09	4.46	5.83	2.29	-0.22
MH C2 80-90	Peat	Peat soil core		80-90	0.09	4.41	5.95	2.17	-0.31
MH C2 90-95	Peat	Peat soil core		90-95	0.09	4.29	6.06	2.32	-0.27
MH C2 95-100	Peat	Peat soil core		95-100	0.09	4.32	5.93	2.17	-0.31
Shallow - Base	Soil DOM	Soil waterDOM	December		0.14	4.30	5.92	2.05	-0.33
Deep	Soil DOM	Soil waterDOM	December		0.14	4.24	5.94	2.03	-0.34
Deep - Base	Soil DOM	Soil waterDOM	December		0.14	4.24	5.78	1.98	-0.33
Shallow	Soil DOM	Soil waterDOM	January		0.15	4.22	5.69	2.10	-0.25
Deep	Soil DOM	Soil waterDOM	January		0.13	3.88	5.06	1.98	-0.19
Dipwell	Soil DOM	Soil waterDOM	January		0.19	3.75	5.53	2.13	-0.19
Shallow	Soil DOM	Soil waterDOM	February		0.13	3.94	5.60	2.09	-0.26
Deep	Soil DOM	Soil waterDOM	February		0.14	3.88	4.61	1.85	-0.13
Dipwell	Soil DOM	Soil waterDOM	February		0.22	4.00	4.62	1.87	-0.06
Shallow	Soil DOM	Soil waterDOM	March		0.15	4.20	5.78	2.04	-0.30
Deep	Soil DOM	Soil waterDOM	March		0.13	4.02	4.82	2.00	-0.10
Dipwell	Soil DOM	Soil waterDOM	March		0.19	4.20	5.03	1.94	-0.14
Deep	Soil POM	Soil waterPOM	December		0.09	4.34	5.57	2.16	-0.23

Shallow	Soil DOM	Soil waterDOM	December	0.15	4.17	6.00	2.06	-0.35	
SPHAG CAP	Veg	Sphagnum	SPHAGsp	0.05	3.66	6.06	2.80	-0.09	
SPHAG GREEN	Veg	Sphagnum	SPHAGsp	0.08	3.80	6.20	2.61	-0.19	
STANDARD	LIGNIN	Standard	STAst	0.06	5.14	6.03	1.81	-0.43	
STANDARD	CELLULOSE	Standard	STAst	0.00	3.60	6.25	3.21	0.05	
	HUMIC								
STANDARD	ACID	Standard	STAst	0.06	2.99	3.68	2.03	0.19	
STANDARD	GLUTEN	Standard	STAst	1.00	3.86	6.55	1.96	0.09	
STANDARD	GLUTEN	Standard	STAst	0.95	3.88	6.83	1.95	-0.02	
STANDARD	GLUTEN	Standard	STAst	0.96	3.89	6.75	1.98	0.02	
STANDARD	GLUTEN	Standard	STAst	*	0.99	3.94	6.83	2.00	0.03

**S3. Table of radiocarbon ages used in this study.**

Site	Type	Depth (cm)	Interval Depth (cm)	DBD (g/cm <sup>3</sup> )	C (%)	<sup>14</sup> C age (BP)
Moor House	Peat core	20-25	22.5	0.181	51.173	655
Moor House	Peat core	30-35	32.5	0.191	50.480	905
Moor House	Peat core	35-40	37.5	0.197	51.913	1030
Moor House	Peat core	45-50	47.5	0.195	51.400	1115
Moor House	Peat core	50-60	55	0.169	52.263	1075
Moor House	Peat core	60-70	65	0.154	51.730	1335
Moor House	Peat core	70-80	75	0.170	53.510	1460
Moor House	Peat core	80-90	85	0.154	52.920	1790
Moor House	Peat core	90-95	92.5	0.114	51.487	1945
Moor House	Peat core	95-100	97.5	0.101	51.897	1895
Moor House	DOM	75				2205
Moor House	DOM	75				2060
Moor House	DOM	First-order stream				>modern
Moor House	DOM	First-order stream				>modern