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# Supporting Information

## **Metal distribution, bioavailability and isotope variations in polluted soils from Lower Swansea Valley, UK**

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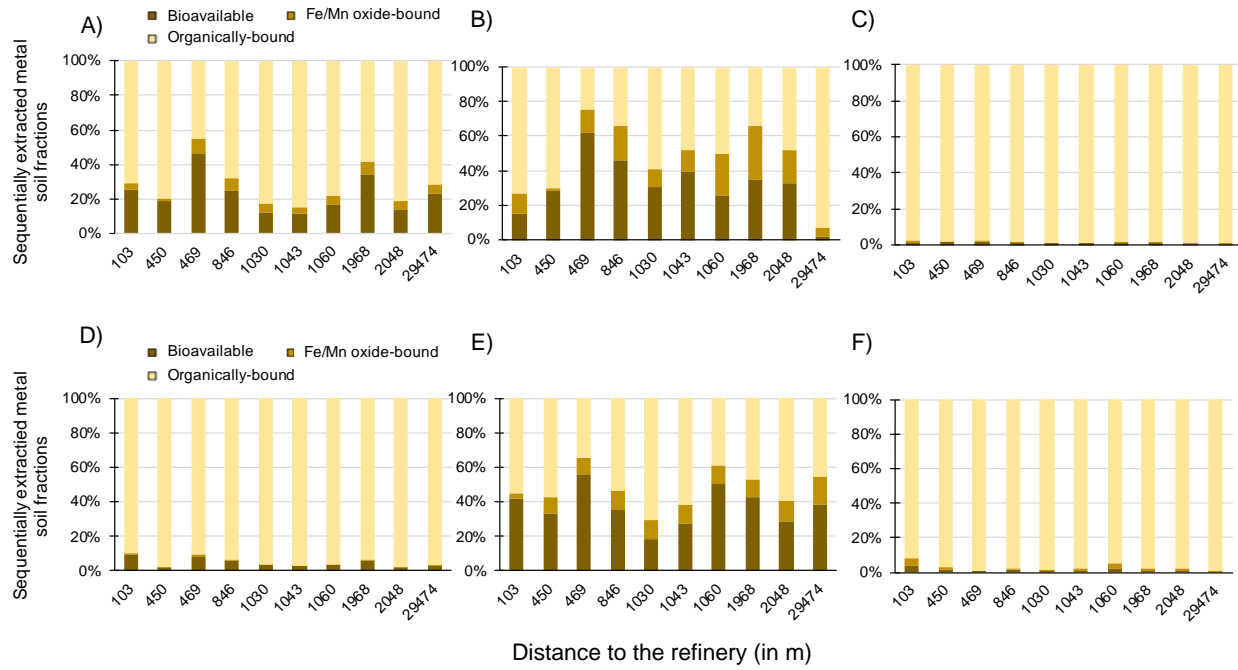
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**Figure S1:** Sequentially extracted soil fractions (%) of A) nickel B) cobalt C) chromium D) copper E) zinc and F) lead with distance to the refinery. The extracted soil fractions include bioavailable, oxide bound and organically bound metals.

**Table S1:** Selected soil properties and sampling location

<b>Sample ID</b>	<b>Land use/Soil description</b>	<b>Distance to refinery (in m)</b>	<b>pH</b>	<b>C<sub>org</sub> (%)</b>
08-C2	nd	29474	nd	10.18
08-09	Rough vegetation	469	5.1	11.6
08-S25	Road verge on the old A 4067	2048	6.42	20.83
09-06	golf course	1060	7.1	8.96
08-19	Garden soil	1043	7	9.6
08-12	Agricultural soil	1030	6.1	7.8
08-S15	Agricultural soil	846	6.37	12.94
08-20	Agricultural soil	1968	5.8	9.5
08/03	Graveyard soil	103	5.05	28.19
08-07	Agricultural soil	450	6.8	22

nd = not determined

**Table S2:** Metal concentration of the reference soil NIST 2711A (Montana soil) from replicate sequential extractions (n = 5).

<b>Soil metal content soil (µg/g)</b>						
	<b>Cr</b>	<b>Co</b>	<b>Ni</b>	<b>Cu</b>	<b>Zn</b>	<b>Pb</b>
<i>Exchangeable and bioavailable bound fraction</i>						
NIST 2711a_1	0.09	0.64	1.00	3.44	34.31	94.65
NIST 2711a_2	0.11	0.77	1.18	3.99	37.77	92.50
NIST 2711a_3	0.11	0.83	1.25	4.11	39.27	97.52
NIST 2711a_4	0.11	0.79	1.21	4.00	38.62	93.49
NIST 2711a_5	0.11	0.89	1.43	4.35	41.78	101.82
<b>Mean</b>	<b>0.11</b>	<b>0.79</b>	<b>1.21</b>	<b>3.98</b>	<b>38.35</b>	<b>96.00</b>
<b>RSD</b>	<b>0.01</b>	<b>0.09</b>	<b>0.15</b>	<b>0.34</b>	<b>2.71</b>	<b>3.76</b>
<i>Reducible fraction (bound to Fe and Mn (hydr)oxides)</i>						
NIST 2711a_1	0.01	0.95	0.38	0.51	13.87	60.83
NIST 2711a_2	0.01	1.01	0.41	0.63	14.83	79.65
NIST 2711a_3	0.01	0.99	0.43	0.64	14.77	81.24
NIST 2711a_4	0.01	1.00	0.42	0.65	15.03	81.35
NIST 2711a_5	0.01	1.00	0.41	0.63	13.41	77.61
<b>Mean</b>	<b>0.01</b>	<b>0.99</b>	<b>0.41</b>	<b>0.61</b>	<b>14.38</b>	<b>76.13</b>
<b>RSD</b>	<b>0.00</b>	<b>0.02</b>	<b>0.02</b>	<b>0.06</b>	<b>0.70</b>	<b>8.69</b>
<i>Oxidizable fraction (bound to organic matter)</i>						
NIST 2711a_1	2.26	1.52	4.08	44.52	92.78	1204.16
NIST 2711a_2	2.23	1.37	3.73	40.72	74.69	1096.89
NIST 2711a_4	2.36	1.40	3.92	47.59	56.36	1037.99
NIST 2711a_5	2.30	1.34	4.03	49.83	53.00	1099.98
<b>Mean</b>	<b>2.29</b>	<b>1.41</b>	<b>3.94</b>	<b>45.67</b>	<b>69.21</b>	<b>1109.75</b>
<b>RSD</b>	<b>0.06</b>	<b>0.08</b>	<b>0.15</b>	<b>3.95</b>	<b>18.38</b>	<b>69.10</b>

**Table S3:** Metal content (Cr, Co, Ni, Cu, Zn and Pb) for the operationally-defined soil fractions (i) water soluble, exchangeable and carbonate-bound (ii) bound to Fe and Mn (hydr)oxides, and (iii) bound to organic matter and sulfides with distance to the Ni refinery in Clydach, Swansea (United Kingdom).

		Soil metal concentration ( $\mu\text{g g}^{-1}$ )					
	Distance to refinery (m)	Cr	Co	Ni	Cu	Zn	Pb
		<i>Bioavailable, exchangeable and carbonate-bound fraction</i>					
Control	29474	0.07	0.11	2.47	0.35	30.03	0.02
08-09	469	0.12	7.69	42.69	22.07	17.22	0.24
08-S25	2048	0.25	12.26	20.13	7.33	286.19	7.07
09-06	1060	0.14	1.01	2.12	2.38	188.32	9.26
08-19	1043	0.13	3.29	6.17	3.45	30.88	0.65
08-12	1030	0.14	1.66	3.36	2.14	13.99	1.29
08-S15	846	0.06	2.43	4.60	12.05	25.43	0.83
08-20	1968	0.15	3.51	23.92	9.48	52.60	0.56
08/03	103	0.15	2.99	42.43	33.66	4.86	4.63
08-07	450	0.71	8.25	43.87	6.80	811.97	3.06
		<i>Reducible fraction (bound to Fe and Mn (hydr)oxides)</i>					
Control	29474	0.01	0.36	0.58	0.03	12.64	0.02
08-09	469	0.06	1.65	8.60	2.70	3.04	0.24
08-S25	2048	0.07	7.05	6.96	0.56	117.61	7.07
09-06	1060	0.02	0.95	0.62	0.16	37.82	9.26
08-19	1043	0.04	0.99	1.98	0.27	12.77	0.65
08-12	1030	0.04	0.53	1.26	0.13	8.10	1.29
08-S15	846	0.02	1.03	1.43	1.29	8.02	0.83
08-20	1968	0.04	3.07	5.55	0.91	12.86	0.56
08/03	103	0.11	2.46	7.15	4.01	0.37	4.63
08-07	450	0.15	0.48	3.34	0.54	230.49	3.06
		<i>Oxidizable fraction (bound to organic matter and sulfides)</i>					
Control	29474	9.06	6.17	7.73	11.20	35.97	8.09
08-09	469	7.29	3.06	42.07	244.22	10.68	40.56
08-S25	2048	31.25	18.05	117.18	328.14	595.80	574.19
09-06	1060	9.30	1.99	9.91	66.75	145.62	348.04
08-19	1043	11.48	4.00	45.33	118.75	71.09	55.70
08-12	1030	12.97	3.19	22.39	62.19	53.53	135.96
08-S15	846	5.16	1.82	12.70	188.90	38.82	62.37
08-20	1968	12.31	3.37	40.89	151.80	57.80	52.42
08/03	103	10.66	14.55	119.41	328.14	6.36	102.99
08-07	450	45.14	20.59	183.51	298.98	1414.96	189.81

**Table S4:** Pollution indices [Pollution index (*PI*); Geoaccumulation index (*I<sub>geo</sub>*)] for the total metal soil content and the bioavailable and exchangeable metal soil content for each metal (Co, Ni, Cu, Zn, Pb and Cr).

<b>Pollution Index (<i>PI</i>)</b>						
<b>Total metal soil content</b>						
Sample ID	Co	Ni	Cu	Zn	Pb	Cr
08-09	1.87	8.66	23.22	0.39	5.17	0.82
08-S25	5.63	13.38	29.00	12.71	71.74	3.45
09-06	0.59	1.17	5.98	4.73	44.05	1.03
08-19	1.25	4.96	10.57	1.46	6.93	1.27
08-12	0.81	2.51	5.56	0.96	16.88	1.44
08-S15	0.79	1.74	17.45	0.92	7.85	0.57
08-20	1.50	6.53	14.00	1.57	6.70	1.37
08/03	3.01	15.68	31.57	0.15	14.22	1.20
08-07	4.42	21.41	26.44	31.25	23.41	5.03
<b>Bioavailable, exchangeable and carbonate bound fraction</b>						
08-09	72.31	17.31	62.49	0.57	10.32	1.56
08-S25	115.19	8.16	20.75	9.53	309.36	3.41
09-06	9.49	0.86	6.73	6.27	405.38	1.86
08-19	30.92	2.50	9.77	1.03	28.61	1.77
08-12	15.65	1.36	6.06	0.47	56.65	1.82
08-S15	22.86	1.86	34.13	0.85	36.12	0.87
08-20	33.03	9.70	26.85	1.75	24.41	2.08
08/03	28.06	17.21	95.30	0.16	202.86	2.04
08-07	77.51	17.79	19.26	27.04	133.84	9.60
Class	Value of <i>PI</i>				Soil pollution*	
1	PI <1				absent	
2	1 < PI < 2				low	
3	2 < PI < 3				moderate	
4	3 < PI < 5				strong	
5	PI >5				very strong	

<b>Geoaccumulation Index (<i>I<sub>geo</sub></i>)</b>						
<b>Total metal soil content</b>						
Sample ID	Co	Ni	Cu	Zn	Pb	Cr
08-09	0.32	2.53	3.95	-1.93	1.79	-0.88
08-S25	1.91	3.16	4.27	3.08	5.58	1.20
09-06	-1.34	-0.35	2.00	1.66	4.88	-0.54
08-19	-0.27	1.73	2.82	-0.04	2.21	-0.24
08-12	-0.89	0.74	1.89	-0.64	3.49	-0.06
08-S15	-0.92	0.21	3.54	-0.71	2.39	-1.39
08-20	0.00	2.12	3.22	0.06	2.16	-0.13
08/03	1.01	3.39	4.40	-3.35	3.24	-0.33
08-07	1.56	3.83	4.14	4.38	3.96	1.75
<b>Bioavailable, exchangeable fraction</b>						
08-09	5.59	3.53	5.38	-1.39	2.78	0.06
08-S25	6.26	2.44	3.79	2.67	7.69	1.18
09-06	2.66	-0.80	2.17	2.06	8.08	0.31
08-19	4.37	0.74	2.70	-0.54	4.25	0.24
08-12	3.38	-0.14	2.02	-1.69	5.24	0.28

08-S15	3.93	0.31	4.51	-0.83	4.59	-0.79
08-20	4.46	2.69	4.16	0.22	4.02	0.47
08/03	4.23	3.52	5.99	-3.21	7.08	0.44
08-07	5.69	3.57	3.68	4.17	6.48	2.68
<b>Class</b>	<b>Value of <math>I_{geo}</math></b>				<b>Soil pollution<sup>#</sup></b>	
1	$I_{geo} > 0$				uncontaminated	
2	$0 < I_{geo} < 1$				uncontaminated to moderately contaminated	
3	$1 < I_{geo} < 2$				moderately contaminated	
4	$2 < I_{geo} < 3$				moderately to heavily contaminated	
5	$3 < I_{geo} < 4$				heavily contaminated	
6	$4 < I_{geo} < 5$				heavily to extremely contaminated	
7	$I_{geo} < 5$				extremely contaminated	

\* after Kowalska et al. (2018)

# after Müller (1969)