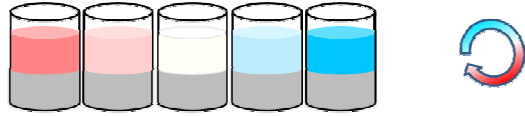


- River sediment Rhine Harbour NL
- own pH River sediment NL
- River sediment Rhine Harbour NL (duplicate)
- own pH River sediment NL
- Modeled at L/S=4.4
- Model at L/S=0.4
- DTL

Object Name pH Dependent Leaching Test Model
River sediment NL

pH Dependent Leaching Test Scenario



Lah Test

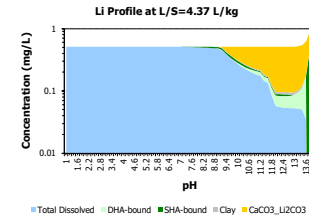
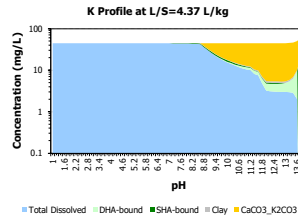
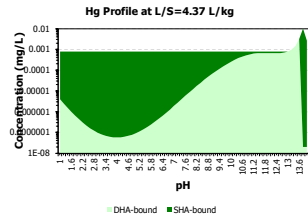
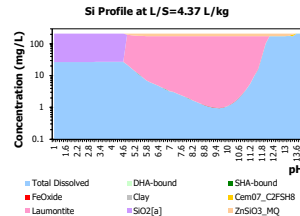
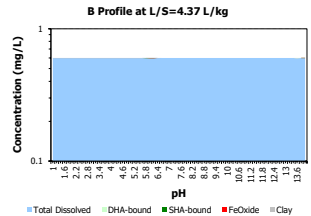
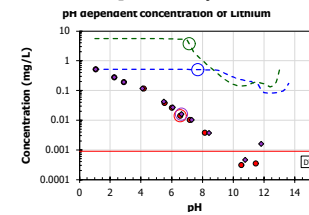
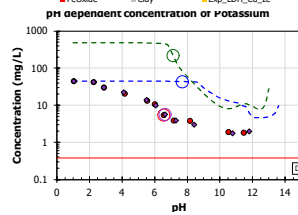
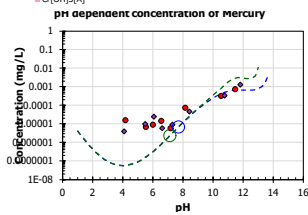
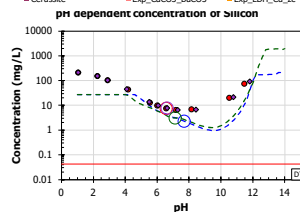
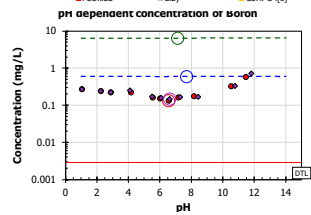
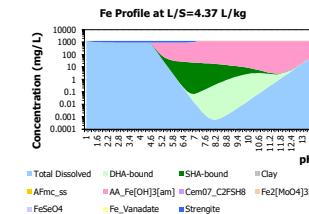
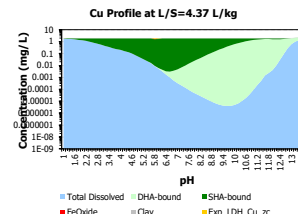
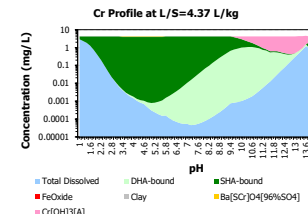
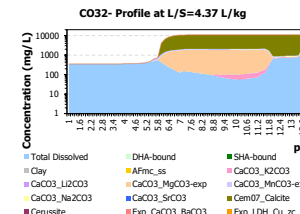
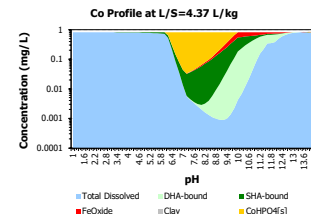
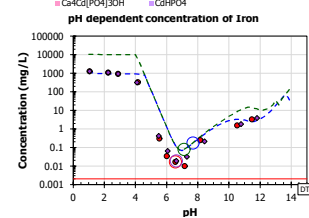
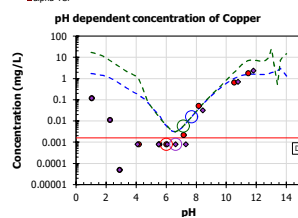
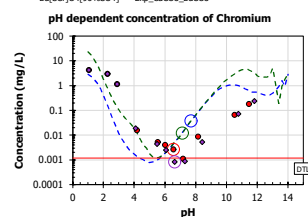
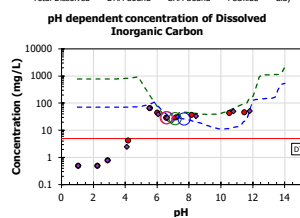
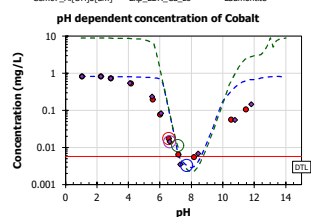
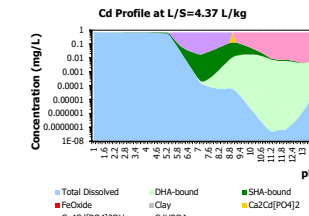
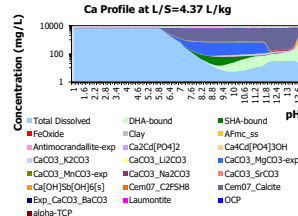
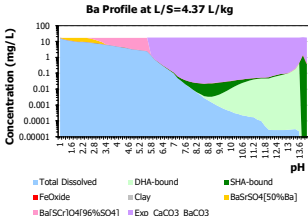
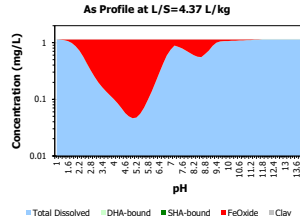
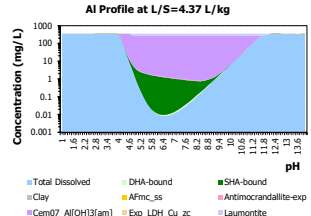
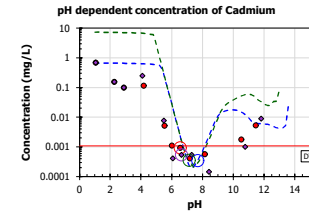
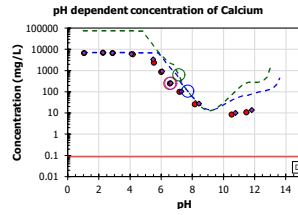
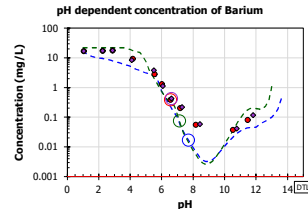
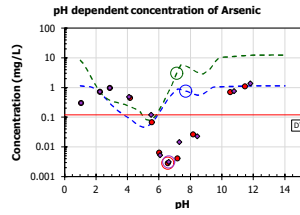
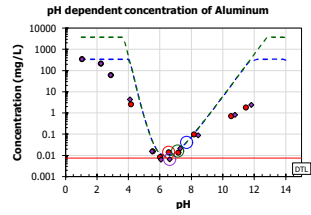
Extra L/S Simulation

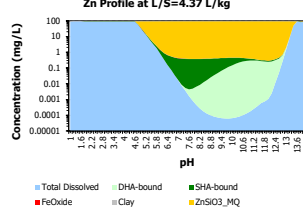
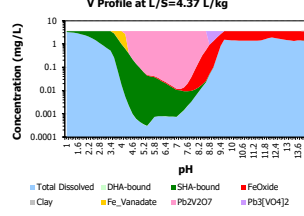
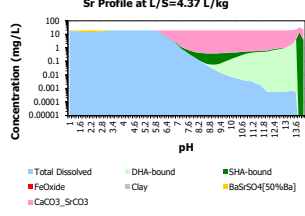
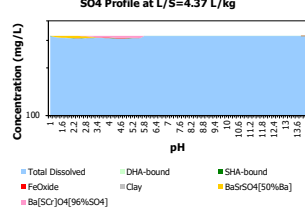
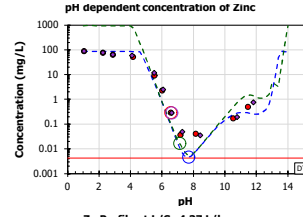
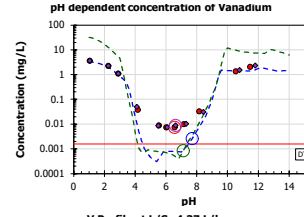
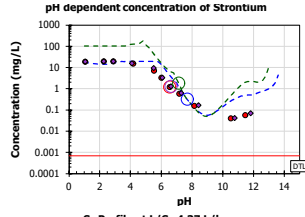
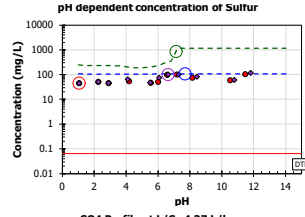
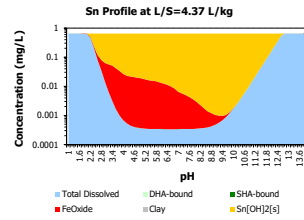
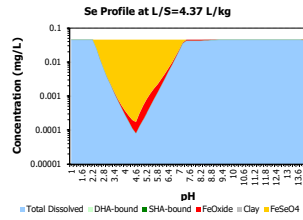
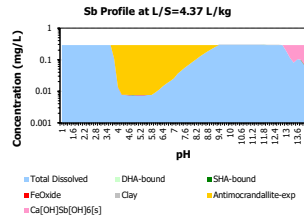
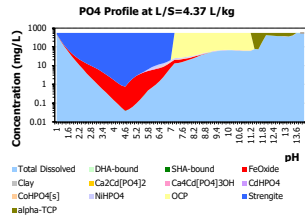
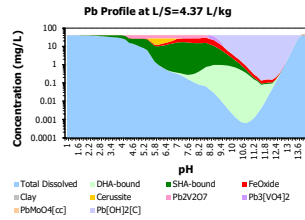
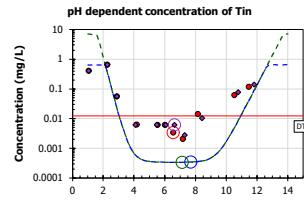
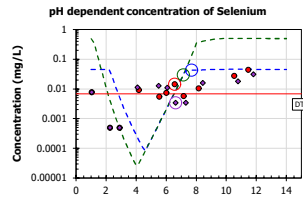
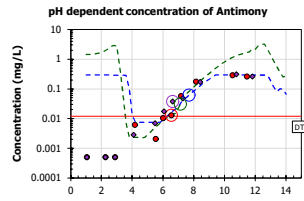
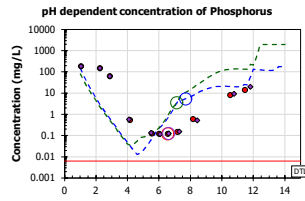
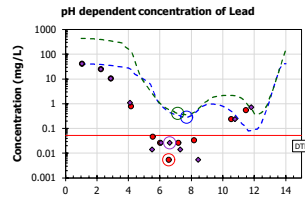
Model Parameters

Entity	Unit	Default	Entity	mg/kg	Entity	mg/kg	Entity	mg/kg
c0		-4.605	Al	1519	B	2.622	PO4	2424
c1		-0.8840	As	5.002	Si	922.6	Sb	1.280
c2		-0.1982	Ba	76.60	Hg	0.003373	Se	0.1988
c3		0.09172	Br	7.990E-09	K	195.0	Sn	2.815
c4		-0.008886	Ca	3.075E+04	Li	2.245	SO4	1402
c5		0.0002645	Cd	2.960	Mg	1580	Sr	84.26
Clay	mg/kg	3000	Cl	3.545E-09	Mn	389.6	V	15.58
Hydrous Ferric Oxid	mg/kg	320.0	Co	3.578	Mo	0.2119	Zn	379.9
L/S	L/kg	4.372	CO32-	4.806E+04	Na	192.4		
pE		2.500	Cr	18.62	Ni	8.431		
pH		8.641	Cu	8.138	NO3	6.200E-09		
Solid Humic Acid	mg/kg	4224	Fe	5571	Pb	180.7		
Simulated Low L/S	L/kg	0.4000						

Minerals

Name	Log(K)	Reaction	Name	Log(K)	Reaction
AA_Fe[OH]3[am]	16.60	AA_Fe[OH]3[am] + 1 H2O -> 1 Fe[OH]4- + 1 H+	CoHPO4[s]	24.48	CoHPO4[s] -> 1 Co+2 + 1 H+ + 1 PO4-3
alpha-TCP	25.50	alpha-TCP -> 3 Ca+2 + 2 PO4-3	Cr[OH]3[A]	68.13	Cr[OH]3[A] + 1 H2O -> 1 CrO4-2 + 5 H+ + 3 e-
Antimocrandallite-e	63.00	Antimocrandallite-exp + 8 H2O -> 3 Al[OH]4- + 1 Ca+2 + 3 H+ + 2 Sb[OH]6-	Exp_CaCO3_BaCO3	21.30	Exp_CaCO3_BaCO3 -> 1 Ba+2 + 2 CO3-2 + 1 Ca+2
Ba[Scr]O4[96%SO4]	9.790	Ba[Scr]O4[96%SO4] -> 1 Ba+2 + 0.04 CrO4-2 + 0.96 SO4-2	Exp_LDH_Cu_zc	58.21	Exp_LDH_Cu_zc + 1 H2O -> 1 Al[OH]4- + 3 CO3-2 + 3 Cu+2 + 1 H+
BaSrSO4[50%Ba]	8.221	BaSrSO4[50%Ba] -> 0.5 Ba+2 + 1 SO4-2 + 0.5 Sr+2	Fe_Vanadate	19.18	Fe_Vanadate + 1 H2O -> 0.5 Fe[OH]4- + 1 VO2+ + 0.5 e-
Ca[OH]Sb[OH]6[s]	2.000	Ca[OH]Sb[OH]6[s] + 1 H+ -> 1 Ca+2 + 1 H2O + 1 Sb[OH]6-	Fe2[MoO4]3[2]	86.35	Fe2[MoO4]3[2] + 8 H2O -> 2 Fe[OH]4- + 8 H+ + 3 MoO4-2
Ca2Cd[PO4]2	32.95	Ca2Cd[PO4]2 -> 2 Ca+2 + 1 Cd+2 + 2 PO4-3	FeSeO4	55.48	FeSeO4 + 2 H2O -> 1 Fe[OH]4- + 4 H+ + 1 SeO4-2 + 1 e-
Ca4Cd[PO4]3OH	39.23	Ca4Cd[PO4]3OH + 1 H+ -> 4 Ca+2 + 1 Cd+2 + 1 H2O + 3 PO4-3	Laumontite	118.0	Laumontite + 8 H2O -> 2 Al[OH]4- + 1 Ca+2 + 8 H+ + 4 H2SiO4-2
CaCO3_K2CO3	19.30	CaCO3_K2CO3 -> 2 CO3-2 + 1 Ca+2 + 2 K+	Manganite	-25.27	Manganite + 3 H+ + 1 e- -> 2 H2O + 1 Mn+2
CaCO3_Li2CO3	21.30	CaCO3_Li2CO3 -> 2 CO3-2 + 1 Ca+2 + 2 Li+	NiHPO4	25.00	NiHPO4 -> 1 H+ + 1 Ni+2 + 1 PO4-3
CaCO3_MgCO3-exp	18.02	CaCO3_MgCO3-exp -> 2 CO3-2 + 1 Ca+2 + 1 Mg+2	OCF	46.90	OCF -> 4 Ca+2 + 1 H+ + 2.5 H2O + 3 PO4-3
CaCO3_MnCO3-exp	20.78	CaCO3_MnCO3-exp -> 2 CO3-2 + 1 Ca+2 + 1 Mn+2	Pb[OH]2[C]	-8.150	Pb[OH]2[C] + 2 H+ -> 2 H2O + 1 Pb+2
CaCO3_Na2CO3	18.30	CaCO3_Na2CO3 -> 2 CO3-2 + 1 Ca+2 + 2 Na+	Pb2V2O7	0.9500	Pb2V2O7 + 3 H+ -> 1.5 H2O + 1 Pb+2 + 1 VO2+
CaCO3_SrCO3	19.85	CaCO3_SrCO3 -> 2 CO3-2 + 1 Ca+2 + 1 Sr+2	Pb3[VO4]2	-3.070	Pb3[VO4]2 + 4 H+ -> 2 H2O + 1.5 Pb+2 + 1 VO2+
CdHPO4	26.48	CdHPO4 -> 1 Cd+2 + 1 H+ + 1 PO4-3	PbMoO4[cc]	13.36	PbMoO4[cc] -> 1 MoO4-2 + 1 Pb+2
Cem07_Al[OH]3[am]	13.76	Cem07_Al[OH]3[am] + 1 H2O -> 1 Al[OH]4- + 1 H+	Sb[OH]3[s]	32.89	Sb[OH]3[s] + 3 H2O -> 3 H+ + 1 Sb[OH]6- + 2 e-
Cem07_Brucite	-16.83	Cem07_Brucite + 2 H+ -> 2 H2O + 1 Mg+2	SiO2[a]	24.64	SiO2[a] + 2 H2O -> 2 H+ + 1 H2SiO4-2
Cem07_C2FSH8	21.41	Cem07_C2FSH8 -> 2 Ca+2 + 2 Fe[OH]4- + 3 H2O + 1 H2SiO4-2	Sn[OH]2[s]	1.447	Sn[OH]2[s] + 2 H+ -> 2 H2O + 1 Sn+2
Cem07_Calcite	8.485	Cem07_Calcite -> 1 CO3-2 + 1 Ca+2	Strengite	47.97	Strengite + 2 H2O -> 1 Fe[OH]4- + 4 H+ + 1 PO4-3
Cem07_Gypsum	4.583	Cem07_Gypsum -> 1 Ca+2 + 2 H2O + 1 SO4-2	ZnSiO3_MQ	18.69	ZnSiO3_MQ + 1 H2O -> 1 H2SiO4-2 + 1 Zn+2
Cerussite	13.20	Cerussite -> 1 CO3-2 + 1 Pb+2			





Legend for Pb Profile:

- Total Dissolved
- DHA-bound
- SHA-bound
- FeOxide
- Clay
- Ca/Ca[PO4]2
- Ca/Ca[PO4]3OH
- CaHPO4
- CoHPO4[s]
- NH4PO4
- OCF
- Strengite
- alpha-TCP
- PbMgO4[cc]
- Pb[OH]2[C]
- Pb3[VO4]2

Legend for PO4 Profile:

- Total Dissolved
- DHA-bound
- SHA-bound
- FeOxide
- Clay
- Ca/Ca[PO4]2
- Ca/Ca[PO4]3OH
- CaHPO4
- CoHPO4[s]
- NH4PO4
- OCF
- Strengite
- alpha-TCP

Legend for Sb Profile:

- Total Dissolved
- DHA-bound
- SHA-bound
- FeOxide
- Clay
- Antimicroandallite-exp
- Ca[OH]Sb(OH)6[s]

Legend for Se Profile:

- Total Dissolved
- DHA-bound
- SHA-bound
- FeOxide
- Clay
- FeSeO4

Legend for Sn Profile:

- Total Dissolved
- DHA-bound
- SHA-bound
- FeOxide
- Clay
- Sn(OH)2[s]

Legend for Sulfur Profile:

- Total Dissolved
- DHA-bound
- SHA-bound
- FeOxide
- Clay
- BaSO4[50%Ba]
- Ba[SO4]96%SO4

Legend for Strontium Profile:

- Total Dissolved
- DHA-bound
- SHA-bound
- FeOxide
- Clay
- BaSrSO4[50%Ba]
- CaCO3_SrCO3

Legend for Vanadium Profile:

- Total Dissolved
- DHA-bound
- SHA-bound
- FeOxide
- Clay
- Fe_Vanadate
- Pb2V2O7
- Pb3[VO4]2

Legend for Zinc Profile:

- Total Dissolved
- DHA-bound
- SHA-bound
- FeOxide
- Clay
- ZnSiO3_MQ

Model Comparison: residuals - Concentration

Name River sediment NL

Legend

Total Average Deviation Square root of the sum of the squared values of residuals divided by the number of values, over the entire X range.

User Average Deviation Square root of the sum of the squared values of residuals divided by the number of values, over the user defined X range.

Fractional Average Deviation Square root of the sum of the squared values of residuals divided by the number of values, over the fraction.

Note that the Total and User Average Deviation columns are averages as well.

Residual details, concentrations

Residuals as log(model/sample)												
Fraction	11	10	9	8	7	6	5	4	3	2	1	Total Avg
pH	1.04	2.25	2.88	4.16	5.53	6.00	6.55	7.16	8.15	10.5	11.5	Deviation
Al	-0.01	0.20	0.74	1.77	0.45	0.17	-0.16	0.10	0.03	1.45	1.98	0.29
As	0.57	-0.03	-0.52	-0.71	-0.02	1.32	2.14	2.32	1.36	0.19	0.01	0.35
Ba	-0.02	-0.26	-0.35	-0.30	-0.04	-0.24	-0.23	-0.56	-0.90	-0.24	-0.27	0.12
Ca	0.02	-0.01	0.02	0.08	0.45	0.73	0.77	0.56	0.24	0.67	0.79	0.15
Cd	-0.01	0.64	0.83	0.74	1.65	1.39	0.39	-0.29	0.29	0.92	0.10	0.25
Cl	-	-	-	-	-	-	-	-	-	-	-	-
Co	-0.01	0.00	0.04	0.18	0.58	0.96	0.78	0.01	-0.25	0.77	0.77	0.16
CO32-	-	-	-	-	-	-	-	-	-	-	-	-
Cr	-0.20	-1.26	-1.82	-1.05	-0.71	-0.33	0.24	1.10	1.00	1.21	0.54	0.30
Cu	1.15	1.99	4.08	2.32	1.35	0.87	-	0.44	-0.14	0.19	-0.05	0.55
F	-	-	-	-	-	-	-	-	-	-	-	-
Fe	-0.04	-0.07	-0.01	0.43	1.54	1.56	0.90	0.91	0.15	0.32	-0.10	0.24
B	0.34	0.39	0.42	0.42	0.57	0.59	0.65	0.56	0.53	0.27	0.02	0.14
Si	-0.90	-0.75	-0.59	-0.21	-0.13	-0.21	-0.24	-0.32	-0.60	-1.07	-0.84	0.19
Hg	-	-	-	-2.44	-1.63	-1.44	-1.26	-0.38	-0.68	0.11	-0.05	0.45
K	-0.01	0.02	0.17	0.33	0.52	0.62	0.91	1.05	1.05	0.84	0.71	0.20
Li	-0.01	0.26	0.43	0.64	1.13	1.29	1.56	1.70	2.12	2.88	2.68	0.49
Mg	-0.01	0.01	0.05	0.17	0.92	0.96	0.72	0.38	0.05	1.39	1.82	0.25
Mn	0.01	-0.01	0.03	0.10	-0.25	-1.35	-1.36	-1.19	-0.66	0.90	0.82	0.24
Mo	1.99	1.89	1.13	0.23	0.20	1.36	0.71	0.60	0.26	0.01	0.24	0.31
Na	0.02	-0.01	0.03	0.10	0.19	0.22	0.28	-0.37	-0.61	-1.01	-1.38	0.17
Ni	-0.01	0.05	0.13	0.32	0.86	0.81	0.59	0.48	0.01	0.87	0.73	0.17
Pb	-0.01	0.19	0.52	1.49	1.90	1.57	1.94	1.12	1.06	0.31	-0.71	0.36
PO4	-	-	-	-	-	-	-	-	-	-	-	-
Sb	2.77	2.77	2.76	0.13	0.56	-0.06	0.11	-0.23	-0.26	0.01	0.05	0.44
Se	0.76	1.89	1.02	-1.68	-0.90	-0.55	-0.29	0.75	0.61	0.22	0.02	0.29
Sn	0.19	-0.23	-0.38	-1.06	-1.25	-1.26	-1.01	-0.79	-1.60	-1.11	-0.48	0.29
SO4	-	-	-	-	-	-	-	-	-	-	-	-
Sr	-0.02	-0.14	-0.08	0.09	0.43	0.62	0.54	0.25	-0.08	0.82	0.92	0.14
Th	-	-	-	-	-	-	-	-	-	-	-	-
U	-	-	-	-	-	-	-	-	-	-	-	-
V	-0.04	-0.06	-0.04	-0.75	-1.34	-0.97	-0.97	-1.01	-0.64	0.00	-0.17	0.22
Zn	-0.01	0.06	0.12	0.20	-0.34	-0.46	-0.51	-0.58	-0.71	0.15	-0.24	0.11
Avg Deviat	0.15	0.19	0.23	0.19	0.18	0.19	0.19	0.17	0.16	0.18	0.18	0.26