

Solute reservoirs reflect variability of early diagenetic processes in temperate brackish surface sediments — Supplementary Material

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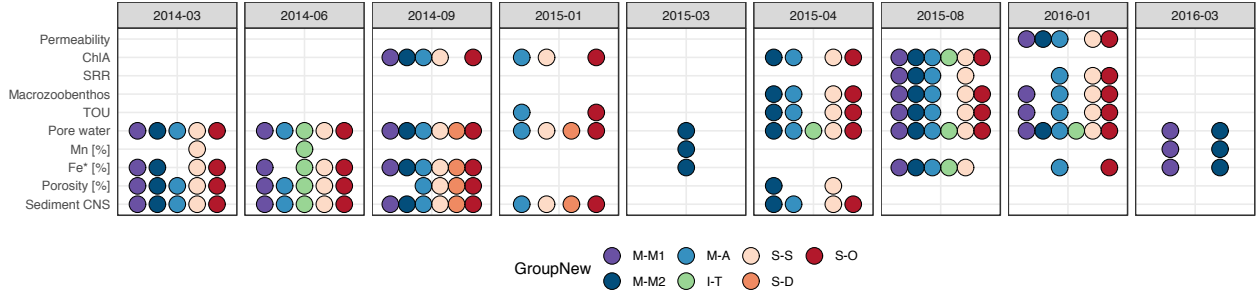
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1 Ship cruise expeditions and parameters

Table 1: Sampled stations and their bottom water temperature, salinity and oxygen measures.

Cruise	Site	Date [UTC]	Long [°]	Lat [°]	Water depth [m]	Sediment type	Temp. [°C]	Salinity	Oxygen [mL/L]
AL434	M-M2	2014-03-28 16:15	11.57330	54.25170	25	mud	5.9	23.5	6.3
AL434	M-M1	2014-03-30 06:09	11.10880	54.10030	23	mud	5.3	21.4	5.7
AL434	S-S	2014-03-31 10:17	11.93900	54.25050	18	sand	5.8	22.4	6.3
AL434	S-O	2014-04-03 08:55	14.05520	54.44230	16	sand	5.6	7.8	8.1
AL434	M-A	2014-04-05 12:23	13.50150	54.83350	45	mud	5.4	20.9	4.3
EMB076	M-M1	2014-06-20 11:41	11.13313	54.13643	17	mud	8.3	20.2	2.5
EMB076	I-T	2014-06-23 06:06	13.58648	54.64532	29	silt	16.1	8.6	6.5
EMB076	S-O	2014-06-25 13:10	14.05472	54.44060	16	sand	15.6	8.2	6.2
EMB076	M-A	2014-06-27 11:36	13.49926	54.83412	46	mud	9.8	16.6	1.9
EMB076	S-S	2014-06-29 05:30	11.94350	54.25017	18	sand	14.3	17.5	5.0
POS475	S-O	2014-09-30 13:04	14.05550	54.44070	16	sand	16.0	8.1	6.2
POS475	M-A	2014-10-02 6:23	13.85310	54.88420	47	mud	15.1	19.0	3.2
POS475	S-D	2014-10-04 8:28	12.69350	54.70280	22	sand	15.1	19.2	3.5
POS475	S-S	2014-10-08 8:36	11.93850	54.25610	18	sand	14.0	22.0	NA
POS475	M-M1	2014-10-09 7:21	11.14350	54.13250	24	mud	14.3	22.7	1.4
POS475	M-M2	2014-10-11 8:04	11.58600	54.22370	27	mud	14.3	23.6	0.3
EMB093	M-A	2015-01-17 09:50	13.85303	54.88368	46	mud	6.9	24.0	6.0
EMB093	S-O	2015-01-19 07:41	14.04867	54.44093	17	sand	4.5	9.5	8.4
EMB093	S-D	2015-01-20 07:47	12.66140	54.67307	20	sand	5.0	13.4	8.0
EMB093	S-S	2015-01-21 09:00	11.93806	54.25697	19	sand	4.8	21.4	7.5
EMB097	M-M2	2015-03-04 9:30	11.66327	54.22526	26	mud	4.3	21.9	6.5
EMB100	S-S	2015-04-09 11:45	11.94395	54.25632	18	sand	5.1	16.2	7.9
EMB100	M-M2	2015-04-10 17:30	11.59004	54.22294	26	mud	4.3	20.5	5.1
EMB100	S-O	2015-04-12 14:35	14.05940	54.44028	15	sand	5.8	8.4	8.6
EMB100	M-A	2015-04-14 11:59	13.85179	54.88540	46	mud	4.7	15.0	6.4
EMB100	I-T	2015-04-15 15:01	13.58469	54.64610	29	silt	6.3	9.2	8.3
EMB111	M-M1	2015-08-25 10:44	11.13590	54.13690	22	mud	13.3	18.1	1.9
EMB111	M-M2	2015-08-28 10:37	11.59580	54.22340	26	mud	12.6	20.4	1.1
EMB111	S-S	2015-08-30 12:18	11.93930	54.25990	19	sand	13.5	18.3	1.6
EMB111	S-O	2015-09-02 06:12	14.06090	54.44260	16	sand	18.3	8.0	5.1
EMB111	I-T	2015-09-03 13:18	13.58360	54.64680	29	silt	16.0	8.6	5.4
EMB111	M-A	2015-09-04 08:26	13.85070	54.88530	46	mud	8.5	12.7	1.7
MSM50b	M-M1	2016-01-16 08:48	11.13880	54.12770	24	mud	3.6	21.5	7.2
MSM50b	M-M2	2016-01-18 17:05	11.59180	54.21420	28	mud	4.0	21.1	7.2
MSM50b	S-S	2016-01-21 00:43	11.93720	54.24170	19	sand	3.9	19.6	7.6
MSM50b	M-A	2016-01-23 08:32	13.85420	54.88550	48	mud	8.3	18.8	4.5
MSM50b	S-O	2016-01-25 03:52	14.06330	54.43300	16	sand	2.0	8.6	9.0
MSM50b	I-T	2016-01-26 21:52	13.59330	54.64080	23	silt	4.3	9.6	7.6
AL472	M-M2	2016-03-03 13:19	11.64790	54.23760	26	mud	4.1	20.6	6.6
AL472	M-M1	2016-03-04 7:02	11.10900	54.10030	23	mud	4.1	20.6	6.6



2 Precision, accuracy and detection limits of used methods

Table 2: Precision, accuracy and detection limits of the used methods to quantify dissolved and solid phase analytes during this study. (nd = not determined, diss. = dissolved, sol. = solid)

Analyte	Phase	Method	Det. limit	Prec. [%]	Acc. [%]	Notes
<i>Fe</i>	diss.	ICP-OES	0.7 µmol/l	6	6	
<i>Mn</i>	diss.	ICP-OES	0.07 µmol/l	6	4	
<i>P</i>	diss.	ICP-OES	4.7 µmol/l	7	8	
<i>S</i>	diss.	ICP-OES	30 µmol/l	10	8	
<i>Si</i>	diss.	ICP-OES	20 µmol/l	5	4	
NH_4^+	diss.	Multianalyser	3.9 µmol/l	4	4	
<i>DIC</i>	diss.	CF-irmMS	nd	4	10	in-house $NaHCO_3$ standard
<i>H_2S</i>	diss.	Photometry	1.2 µmol/l	nd	nd	
<i>Fe*</i>	sol.	Photometry	56 - 280 ppb	1	nd	Extraction of 0.2 - 1.0 g freeze dried sediment in 10 mL HCl solution
<i>TC</i>	sol.	Elemental Analyser	nd	2	3	in-house sediment standard
<i>TN</i>	sol.	Elemental Analyser	nd	10	5	in-house sediment standard
<i>TS</i>	sol.	Elemental Analyser	nd	10	1	in-house sediment standard
<i>TIC</i>	sol.	Elemental Analyser	nd	9	13	in-house sediment standard

3 PCA with benthic solute reservoirs of the top 15 cm

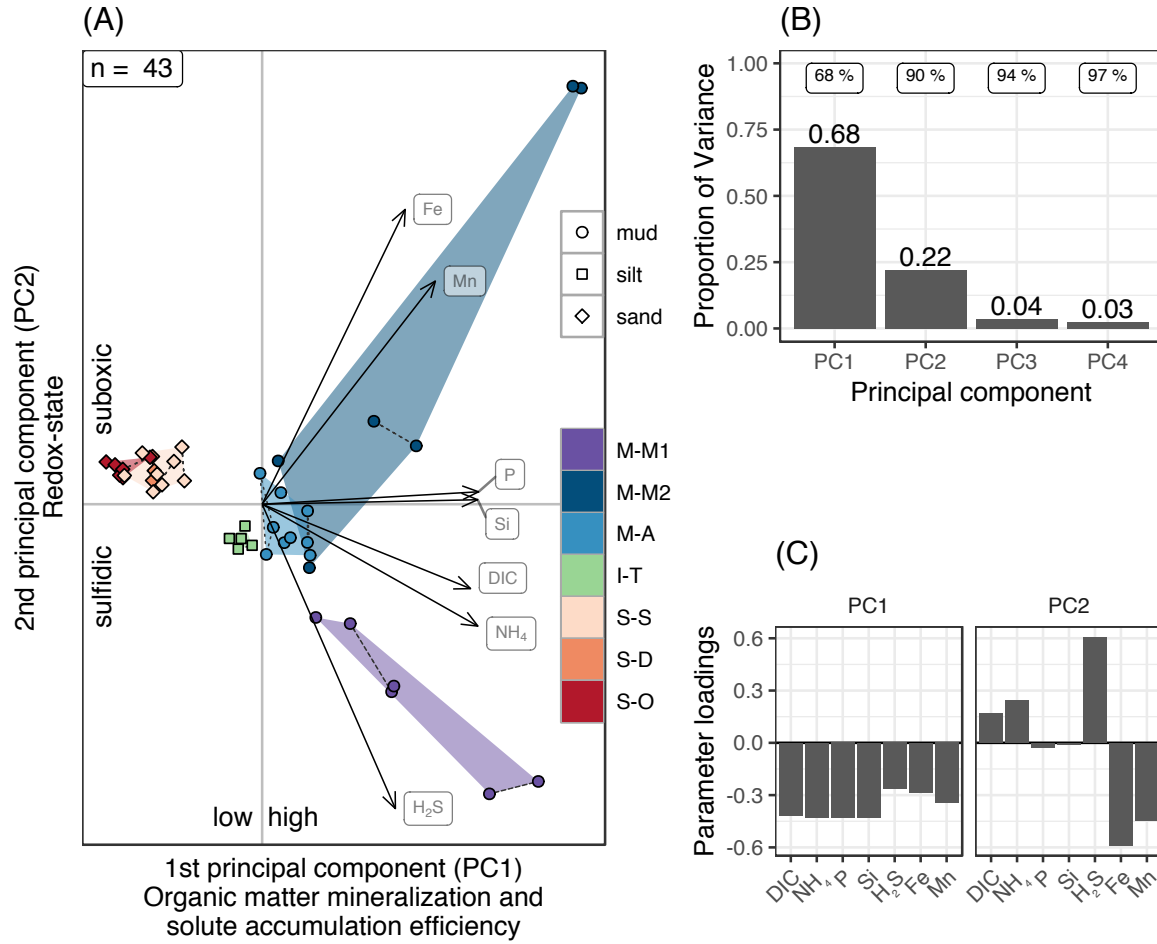
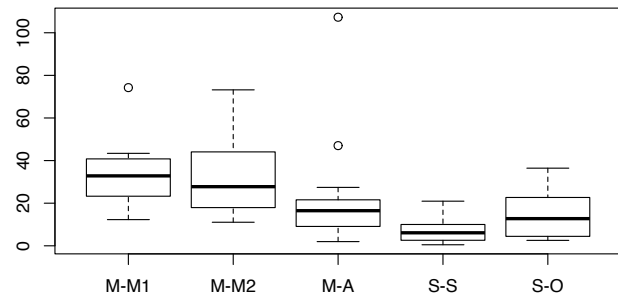
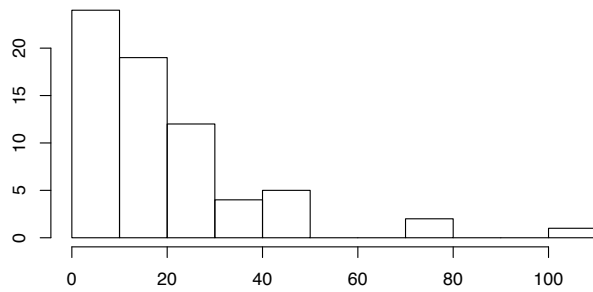


Figure 1: Principal component analysis (PCA) of southern Baltic Sea benthic solute reservoirs in the top 15 cm. A) Each dot represents the mean benthic solute reservoir of DIC , NH_4^+ , PO_4 , H_4SiO_4 , sulfide, Fe^{2+} , and Mn^{2+} from parallel cores of each sampling campaign. Shaded areas envelop the expansion of variability of each study site in the two-dimensional space. B) Explained variance by different principal components. The first principal component alone explains 68 %, already, and cumulative proportions of the first two principal components explain 90 % of the total variance. C) Loadings of the major two components of the principal component analysis. All considered parameters substantially contribute to PC1. PC2 is loaded with the redox sensitive parameters dissolved sulfide (H_2S), Fe^{2+} and Mn^{2+} (note the anticorrelation between H_2S and dissolved metals Fe^{2+} and Mn^{2+}) with minor contributions of DIC and NH_4^+ .

4 Statistical tests

4.1 SRR in top 15 cm vs site



```
#####
Shapiro-Wilk normality test

data: resid(lm(data ~ factor))
W = 0.77739, p-value = 1.066e-08

=> Residuals are rejected to be normal distributed (Shapiro-Wilks's p-value < 0.05 )

#####
Kruskal-Wallis rank sum test

data: data and factor
Kruskal-Wallis chi-squared = 28.2266, df = 4, p-value = 0

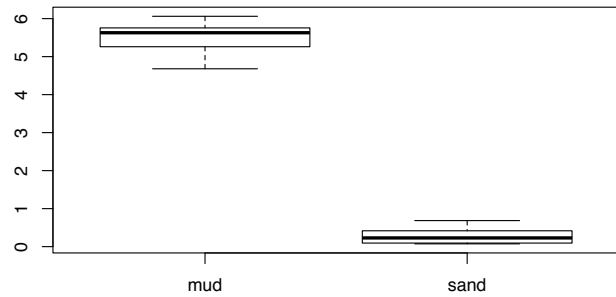
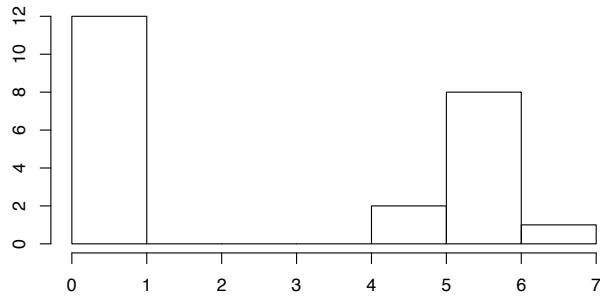
Comparison of data by factor
(No adjustment)
Col Mean-|
Row Mean |
-----|-----
M-M1 | -1.775081
      | 0.0379
M-M2 | -1.861791 0.120506
      | 0.0313 0.4520
S-O | 0.742935 2.151263 2.237785
      | 0.2288 0.0157* 0.0126*
S-S | 3.194668 4.039926 4.420054 1.858455
      | 0.0007* 0.0000* 0.0000* 0.0316

alpha = 0.05
Reject Ho if p <= alpha/2
Table above shows Dunn's test z-statistic (upper line) and p-value (lower line)

#####
Data summary
factor x.mean x.sd x.median x.n
1 M-M1 35.357412 20.541142 32.825099 7
2 M-M2 32.800403 19.248148 27.752536 10
3 M-A 21.005840 21.939272 16.477328 21
4 S-S 7.096812 5.665436 6.107501 19
5 S-O 15.259948 11.447795 12.752338 10
```

4.2 Solid phase parameters in top 15 cm

4.2.1 TOC by sediment type



```
#####
Shapiro-Wilk normality test

data: resid(lm(data ~ factor))
W = 0.96385, p-value = 0.5453

=> Residuals are accepted as normal distributed (Shapiro-Wilks's p-value > 0.05 )

#####
Bartlett test of homogeneity of variances

data: data and factor
Bartlett's K-squared = 3.8945, df = 1, p-value = 0.04844

=> Group variances are rejected to be equal (Bartlett's p-value < 0.05 )

#####
Kruskal-Wallis rank sum test

data: data and factor
Kruskal-Wallis chi-squared = 16.5, df = 1, p-value = 0

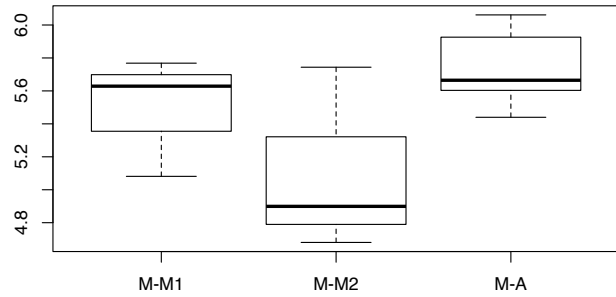
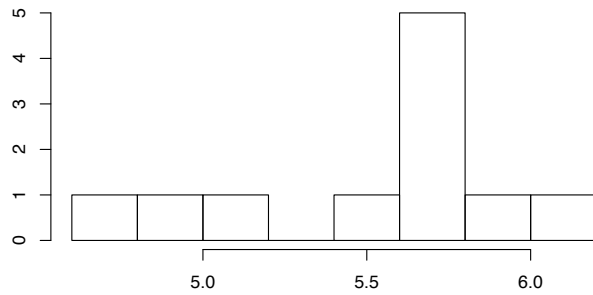
Comparison of data by factor
(No adjustment)

Col Mean |
Row Mean |      mud
-----+-----
sand |    4.062019
      |    0.0000*

alpha = 0.05
Reject Ho if p <= alpha/2
Table above shows Dunn's test z-statistic (upper line) and p-value (lower line)

#####
Data summary
factor  x.mean      x.sd  x.median x.n
1  mud 5.4996771 0.4352710 5.6287143 11
2  sand 0.2821053 0.2299427 0.2290667 12
```

4.2.2 TOC by site within muds



```
#####
Shapiro-Wilk normality test

data: resid(lm(data ~ factor))
W = 0.95108, p-value = 0.6578

=> Residuals are accepted as normal distributed (Shapiro-Wilks's p-value > 0.05 )

#####
Bartlett test of homogeneity of variances

data: data and factor
Bartlett's K-squared = 1.5775, df = 2, p-value = 0.4544

=> Group variances are accepted as equal (Bartlett's p-value > 0.05 )

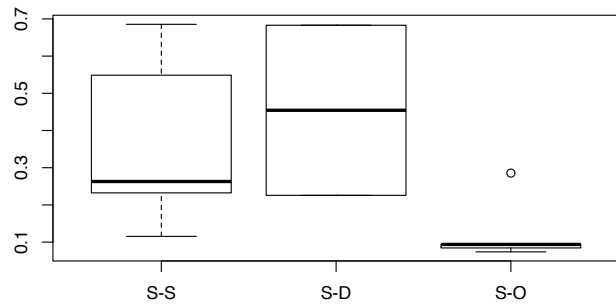
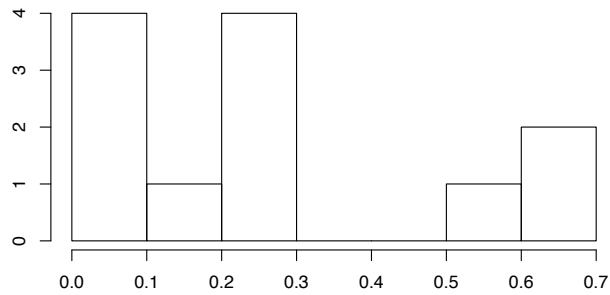
#####
ANOVA
          Df Sum Sq Mean Sq F value Pr(>F)
factor      2  0.7476    0.3738    2.607  0.134
Residuals   8  1.1470    0.1434
Tukey multiple comparisons of means
 95% family-wise confidence level

Fit: aov(formula = data ~ factor)

$factor
      diff      lwr      upr    p adj
M-M2-M-M1 -0.3851048 -1.2685312  0.4983217 0.4616786
M-A-M-M1   0.2462552 -0.5439054  1.0364159 0.6608648
M-A-M-M2   0.6313600 -0.1588006  1.4215206 0.1161219

#####
Data summary
 factor  x.mean      x.sd x.median x.n
1  M-M1  5.492771  0.3631467  5.628714   3
2  M-M2  5.107667  0.5616279  4.899133   3
3  M-A   5.739027  0.2511998  5.664667   5
```

4.2.3 TOC by site within sands



```
#####
Shapiro-Wilk normality test

data: resid(lm(data ~ factor))
W = 0.93478, p-value = 0.4335

=> Residuals are accepted as normal distributed (Shapiro-Wilks's p-value > 0.05 )

#####
Bartlett test of homogeneity of variances

data: data and factor
Bartlett's K-squared = 3.3854, df = 2, p-value = 0.184

=> Group variances are accepted as equal (Bartlett's p-value > 0.05 )

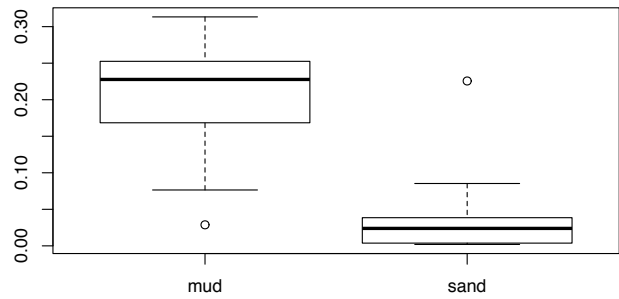
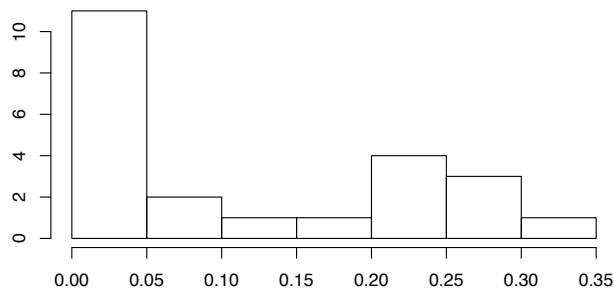
#####
ANOVA
      Df Sum Sq Mean Sq F value Pr(>F)
factor    2  0.2184  0.10921    2.706   0.12
Residuals  9  0.3632  0.04035
Tukey multiple comparisons of means
 95% family-wise confidence level

Fit: aov(formula = data ~ factor)

$factor
      diff      lwr      upr    p adj
S-D-S-S  0.08538727 -0.3838709  0.5546455  0.8693513
S-O-S-S -0.24265273 -0.5973786  0.1120731  0.1913299
S-O-S-D -0.32804000 -0.7972982  0.1412182  0.1800614

#####
Data summary
      factor  x.mean      x.sd  x.median x.n
1  S-S  0.3689794  0.23806319  0.2629333   5
2  S-D  0.4543667  0.32333636  0.4543667   2
3  S-O  0.1263267  0.08937106  0.0938000   5
```

4.2.4 TIC by sediment type



```
#####
Shapiro-Wilk normality test

data: resid(lm(data ~ factor))
W = 0.94603, p-value = 0.2417

=> Residuals are accepted as normal distributed (Shapiro-Wilks's p-value > 0.05 )

#####
Bartlett test of homogeneity of variances

data: data and factor
Bartlett's K-squared = 1.0512, df = 1, p-value = 0.3052

=> Group variances are accepted as equal (Bartlett's p-value > 0.05 )

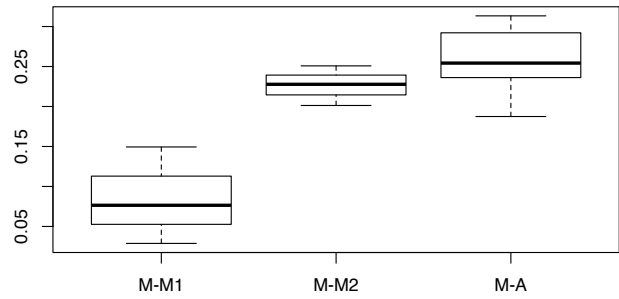
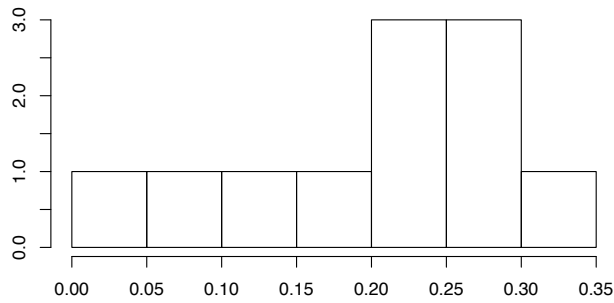
#####
ANOVA
      Df Sum Sq Mean Sq F value    Pr(>F)
factor    1  0.1493   0.14926    26.14 4.6e-05 ***
Residuals 21  0.1199   0.00571
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
Tukey multiple comparisons of means
 95% family-wise confidence level

Fit: aov(formula = data ~ factor)

$factor
      diff      lwr      upr    p adj
sand-mud -0.1612694 -0.226868 -0.09567085 4.6e-05

#####
Data summary
 factor  x.mean      x.sd  x.median x.n
1   mud 0.20161688 0.08729168 0.22773333 11
2  sand 0.04034747 0.06304458 0.02386667 12
```


4.2.5 TIC by site within muds



```
#####
Shapiro-Wilk normality test

data: resid(lm(data ~ factor))
W = 0.96815, p-value = 0.8672

=> Residuals are accepted as normal distributed (Shapiro-Wilks's p-value > 0.05 )

#####
Bartlett test of homogeneity of variances

data: data and factor
Bartlett's K-squared = 1.2151, df = 2, p-value = 0.5447

=> Group variances are accepted as equal (Bartlett's p-value > 0.05 )

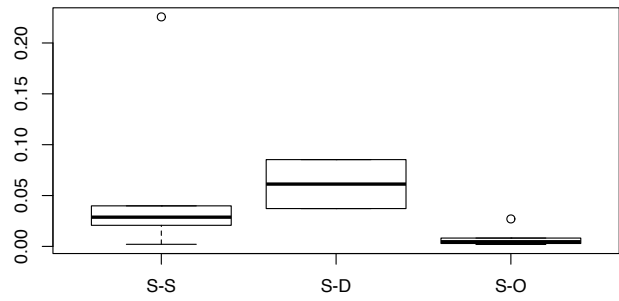
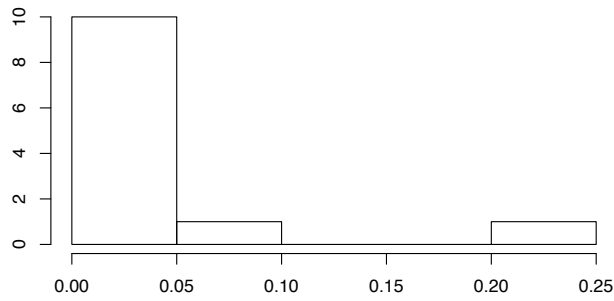
#####
ANOVA
      Df Sum Sq Mean Sq F value Pr(>F)
factor    2  0.05790  0.028952   12.66 0.00332 **
Residuals  8  0.01829  0.002287
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
Tukey multiple comparisons of means
 95% family-wise confidence level

Fit: aov(formula = data ~ factor)

$factor
      diff      lwr      upr    p adj
M-M2-M-M1 0.14171587  0.03014771 0.2532840 0.0163826
M-A-M-M1   0.17178254  0.07199294 0.2715721 0.0029511
M-A-M-M2   0.03006667 -0.06972293 0.1298563 0.6781013

#####
Data summary
 factor  x.mean      x.sd  x.median x.n
1  M-M1 0.08488413 0.06074613 0.07646667  3
2  M-M2 0.22660000 0.02478611 0.22773333  3
3   M-A 0.25666667 0.04920623 0.25426667  5
```

4.2.6 TIC by site within sands



```
#####
Shapiro-Wilk normality test

data: resid(lm(data ~ factor))
W = 0.74889, p-value = 0.002602

=> Residuals are rejected to be normal distributed (Shapiro-Wilks's p-value < 0.05 )

#####
Kruskal-Wallis rank sum test

data: data and factor
Kruskal-Wallis chi-squared = 4.7538, df = 2, p-value = 0.09

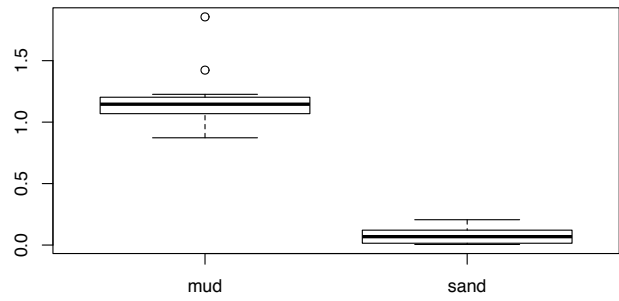
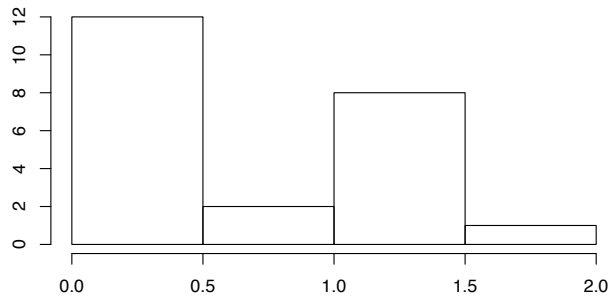
Comparison of data by factor
(No adjustment)

Col Mean-|
Row Mean |      S-D      S-O
-----|-----
S-O | 1.988980
    | 0.0234*
    |
S-S | 0.795592 -1.578704
    | 0.2131  0.0572

alpha = 0.05
Reject Ho if p <= alpha/2
Table above shows Dunn's test z-statistic (upper line) and p-value (lower line)

#####
Data summary
factor    x.mean    x.sd    x.median x.n
1 S-S 0.06340727 0.09173120 0.02873333 5
2 S-D 0.06126667 0.03403541 0.06126667 2
3 S-O 0.00892000 0.01038657 0.00460000 5
```

4.2.7 TS by sediment type



```
#####
Shapiro-Wilk normality test

data: resid(lm(data ~ factor))
W = 0.78712, p-value = 0.0002401

=> Residuals are rejected to be normal distributed (Shapiro-Wilks's p-value < 0.05 )

#####
Kruskal-Wallis rank sum test

data: data and factor
Kruskal-Wallis chi-squared = 16.5, df = 1, p-value = 0

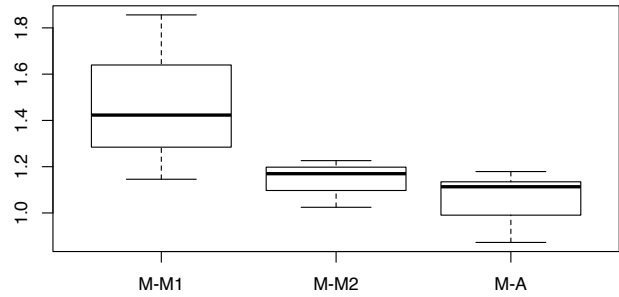
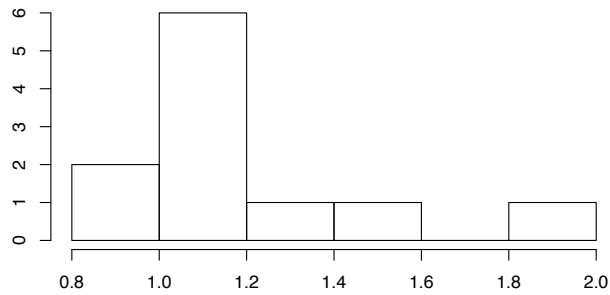
Comparison of data by factor
(No adjustment)

Col Mean-|
Row Mean |      mud
-----|-----
sand | 4.062019
      | 0.0000*

alpha = 0.05
Reject Ho if p <= alpha/2
Table above shows Dunn's test z-statistic (upper line) and p-value (lower line)

#####
Data summary
factor  x.mean  x.sd x.median x.n
1  mud 1.1941212 0.26046880 1.145733 11
2  sand 0.0764298 0.06732417 0.068300 12
```

4.2.8 TS by site within muds



```
#####
Shapiro-Wilk normality test

data: resid(lm(data ~ factor))
W = 0.96459, p-value = 0.8273

=> Residuals are accepted as normal distributed (Shapiro-Wilks's p-value > 0.05 )

#####
Bartlett test of homogeneity of variances

data: data and factor
Bartlett's K-squared = 3.8251, df = 2, p-value = 0.1477

=> Group variances are accepted as equal (Bartlett's p-value > 0.05 )

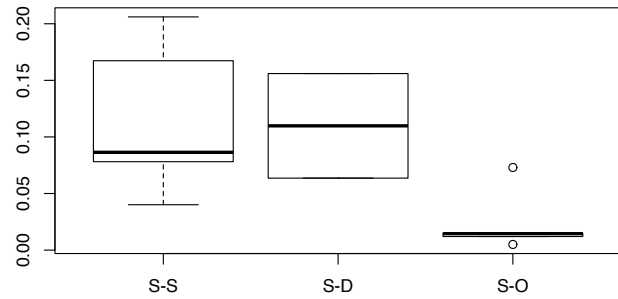
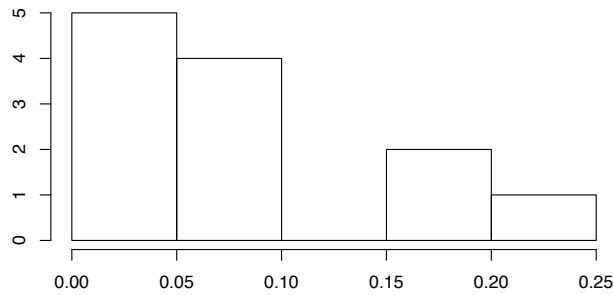
#####
ANOVA
      Df Sum Sq Mean Sq F value Pr(>F)
factor    2  0.3380   0.16899    3.971  0.0634 .
Residuals  8  0.3405   0.04256
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
Tukey multiple comparisons of means
 95% family-wise confidence level

Fit: aov(formula = data ~ factor)

$factor
      diff      lwr      upr    p adj
M-M2-M-M1 -0.33480000 -0.8161008  0.14650082  0.1773119
M-A-M-M1   -0.41695556 -0.8474441  0.01353298  0.0570617
M-A-M-M2   -0.08215556 -0.5126441  0.34833298  0.8516642

#####
Data summary
 factor  x.mean      x.sd x.median x.n
1  M-M1  1.474956  0.3579982  1.423067   3
2  M-M2  1.140156  0.1040360  1.169733   3
3   M-A  1.058000  0.1249820  1.113267   5
```

4.2.9 TS by site within sands



```
#####
Shapiro-Wilk normality test

data: resid(lm(data ~ factor))
W = 0.93865, p-value = 0.4807

=> Residuals are accepted as normal distributed (Shapiro-Wilks's p-value > 0.05 )

#####
Bartlett test of homogeneity of variances

data: data and factor
Bartlett's K-squared = 2.4432, df = 2, p-value = 0.2948

=> Group variances are accepted as equal (Bartlett's p-value > 0.05 )

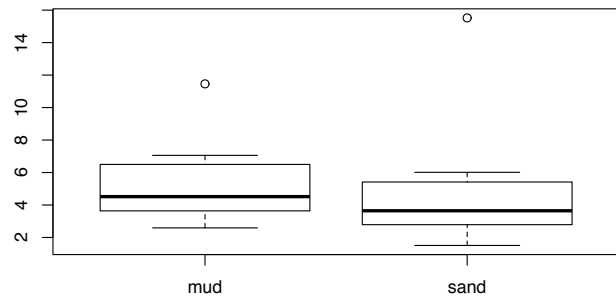
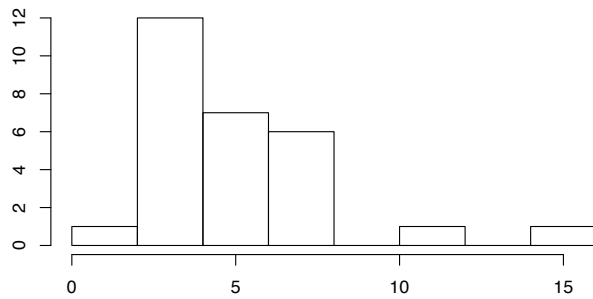
#####
ANOVA
      Df Sum Sq Mean Sq F value Pr(>F)
factor    2  0.02369  0.011847   4.075 0.0549 .
Residuals  9  0.02616  0.002907
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
Tukey multiple comparisons of means
 95% family-wise confidence level

Fit: aov(formula = data ~ factor)

$factor
      diff      lwr      upr    p adj
S-D-S-S -0.005804848 -0.1317543  0.120144614 0.9909219
S-U-S-S -0.091698182 -0.1869070  0.003510663 0.0587027
S-U-S-D -0.085893333 -0.2118428  0.040056129 0.1929474

#####
Data summary
  factor    x.mean      x.sd  x.median x.n
1   S-S 0.11560485 0.06859040 0.08640000  5
2   S-D 0.10980000 0.06533667 0.10980000  2
3   S-U 0.02390667 0.02773344 0.01453333  5
```

4.3 TOU vs Sediment type



```
#####
Shapiro-Wilk normality test

data: resid(lm(data ~ factor))
W = 0.78098, p-value = 5.022e-05

=> Residuals are rejected to be normal distributed (Shapiro-Wilks's p-value < 0.05 )

#####
Kruskal-Wallis rank sum test

data: data and factor
Kruskal-Wallis chi-squared = 1.3282, df = 1, p-value = 0.25

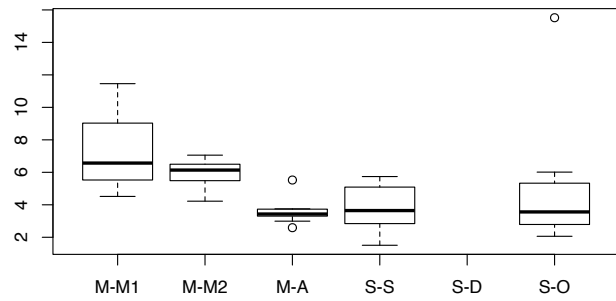
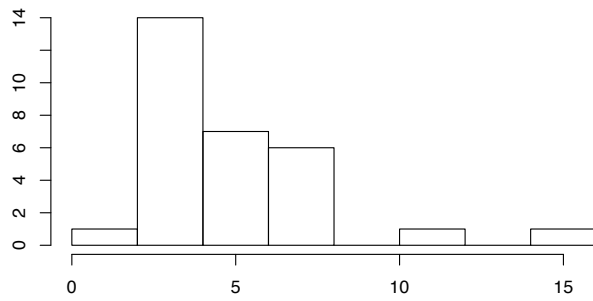
Comparison of data by factor
(No adjustment)

Col Mean-|
Row Mean |      mud
-----|-----
sand | 1.152489
      | 0.1246

alpha = 0.05
Reject Ho if p <= alpha/2
Table above shows Dunn's test z-statistic (upper line) and p-value (lower line)

#####
Data summary
factor  x.mean    x.sd x.median x.n
1  mud 5.139303 2.179531 4.515585 17
2  sand 4.851183 3.836256 3.644933 11
```

4.4 TOU vs site



```
#####
Shapiro-Wilk normality test

data: resid(lm(data ~ factor))
W = 0.78155, p-value = 3.077e-05

=> Residuals are rejected to be normal distributed (Shapiro-Wilks's p-value < 0.05 )

#####
Kruskal-Wallis rank sum test

data: data and factor
Kruskal-Wallis chi-squared = 11.2638, df = 4, p-value = 0.02

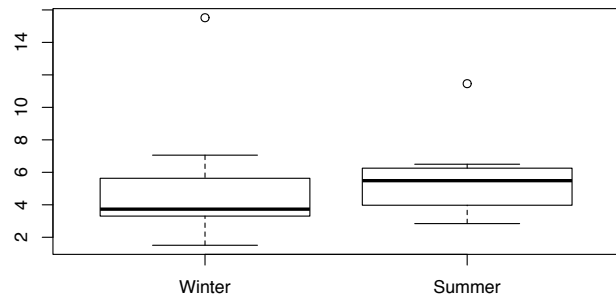
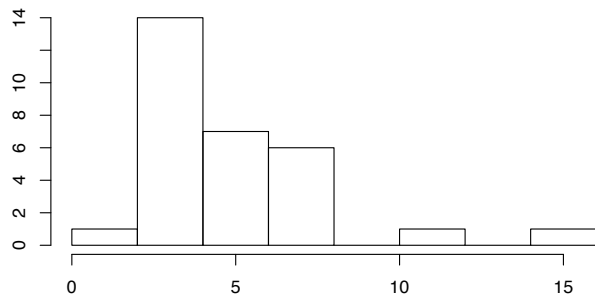
      Comparison of data by factor
      (No adjustment)

Col Mean-|
Row Mean |      M-A      M-M1      M-M2      S-O
-----|-----
M-M1 | -2.620153
      | 0.0044*
M-M2 | -2.385006  0.364067
      | 0.0085*   0.3579
S-O  | -0.604652  2.025900  1.751505
      | 0.2727   0.0214*  0.0399
S-S  | -0.226281  2.159002  1.903816  0.304850
      | 0.4105   0.0154*  0.0285   0.3802

alpha = 0.05
Reject Ho if p <= alpha/2
Table above shows Dunn's test z-statistic (upper line) and p-value (lower line)

#####
Data summary
factor  x.mean  x.sd x.median x.n
1 M-M1  7.278429 2.9507976 6.569346 4
2 M-M2  5.880409 1.0880982 6.138080 5
3 M-A   3.587087 0.8163357 3.431390 9
4 S-S   3.764980 1.7039902 3.644933 5
5 S-O   5.340099 4.6907052 3.561476 7
```

4.5 TOU vs season



```
#####
Shapiro-Wilk normality test

data: resid(lm(data ~ factor))
W = 0.78222, p-value = 3.161e-05

=> Residuals are rejected to be normal distributed (Shapiro-Wilks's p-value < 0.05 )

#####
Kruskal-Wallis rank sum test

data: data and factor
Kruskal-Wallis chi-squared = 1.0104, df = 1, p-value = 0.31

Comparison of data by factor
(No adjustment)

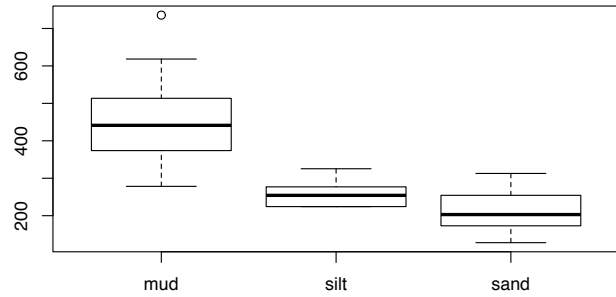
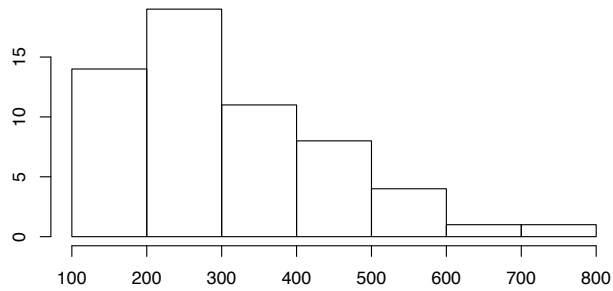
Col Mean-|
Row Mean | Summer
-----|-----
Winter | 1.005195
      | 0.1574

alpha = 0.05
Reject Ho if p <= alpha/2
Table above shows Dunn's test z-statistic (upper line) and p-value (lower line)

#####
Data summary
factor x.mean x.sd x.median x.n
1 Winter 4.641667 2.823016 3.731262 23
2 Summer 5.749542 2.847504 5.486150 7
```


4.6 Benthic solute reservoirs vs sediment type

4.6.1 DIC



```
#####
Shapiro-Wilk normality test
data: resid(lm(data ~ factor))
W = 0.96396, p-value = 0.08253

=> Residuals are accepted as normal distributed (Shapiro-Wilks's p-value > 0.05 )

#####
Bartlett test of homogeneity of variances
data: data and factor
Bartlett's K-squared = 15.921, df = 2, p-value = 0.000349

=> Group variances are rejected to be equal (Bartlett's p-value < 0.05 )

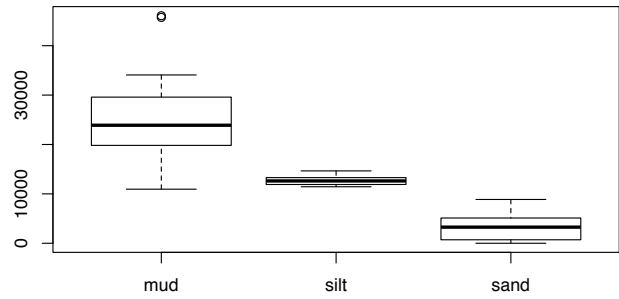
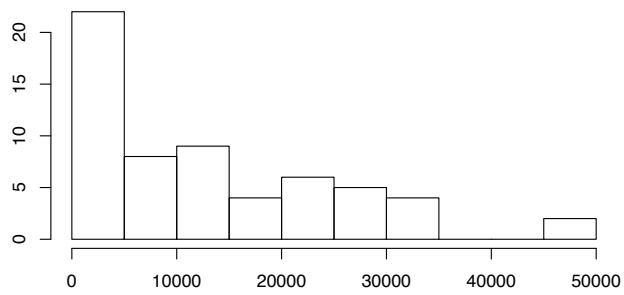
#####
Kruskal-Wallis rank sum test
data: data and factor
Kruskal-Wallis chi-squared = 41.3445, df = 2, p-value = 0

Comparison of data by factor
(No adjustment)
Col Mean-|
Row Mean |      mud      sand
-----|-----
sand | 6.405388
      | 0.0000*
      |
silt | 2.632624 -1.289693
      | 0.0042*  0.0986

alpha = 0.05
Reject Ho if p <= alpha/2
Table above shows Dunn's test z-statistic (upper line) and p-value (lower line)

#####
Data summary
factor  x.mean    x.sd x.median x.n
1  mud 447.6866 112.03728 441.2883 24
2  silt 259.9203  38.77795 254.2988  6
3  sand 210.4122  53.70576 203.0143 28
```

4.6.2 NH_4^+



```
#####
Shapiro-Wilk normality test

data: resid(lm(data ~ factor))
W = 0.88266, p-value = 3.252e-05

=> Residuals are rejected to be normal distributed (Shapiro-Wilks's p-value < 0.05 )

#####
Kruskal-Wallis rank sum test

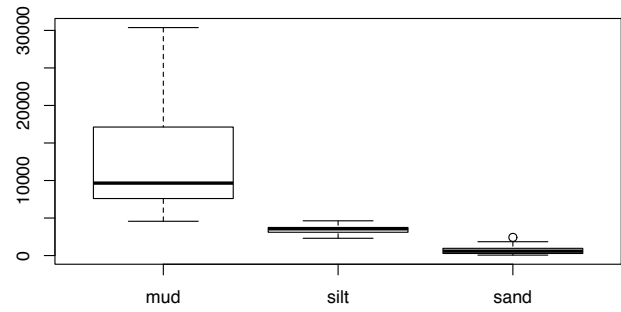
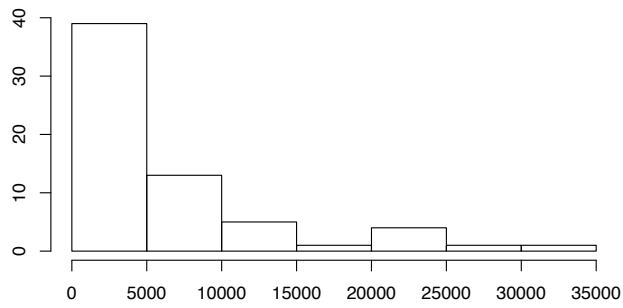
data: data and factor
Kruskal-Wallis chi-squared = 47.2133, df = 2, p-value = 0

Comparison of data by factor
(No adjustment)
Col Mean-|
Row Mean |      mud      sand
-----|-----
sand | 6.822391
      | 0.0000*
      |
silt | 1.717839 -2.738023
      | 0.0429  0.0031*

alpha = 0.05
Reject Ho if p <= alpha/2
Table above shows Dunn's test z-statistic (upper line) and p-value (lower line)

#####
Data summary
factor  x.mean  x.sd  x.median x.n
1  mud 25084.551 8975.596 23895.244 23
2  silt 12727.192 1114.550 12617.700 7
3  sand 3324.075 2724.181 3263.194 30
```

4.6.3 PO₄



```
#####
Shapiro-Wilk normality test

data: resid(lm(data ~ factor))
W = 0.78495, p-value = 2.793e-08

=> Residuals are rejected to be normal distributed (Shapiro-Wilks's p-value < 0.05 )

#####
Kruskal-Wallis rank sum test

data: data and factor
Kruskal-Wallis chi-squared = 51.9694, df = 2, p-value = 0

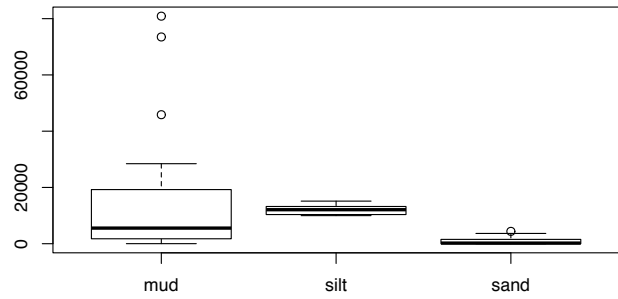
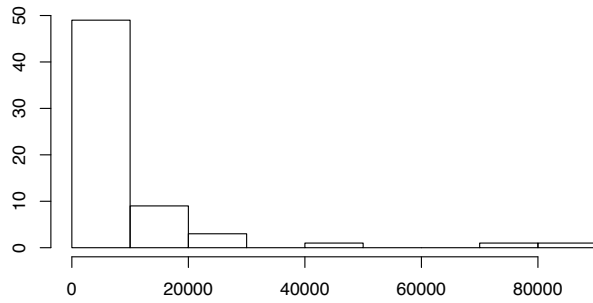
      Comparison of data by factor
      (No adjustment)

Col Mean-|
Row Mean |      mud      sand
-----|-----
sand |      7.201662
      |      0.0000*
      |
silt |      2.253208      -2.560052
      |      0.0121*      0.0052*

alpha = 0.05
Reject Ho if p <= alpha/2
Table above shows Dunn's test z-statistic (upper line) and p-value (lower line)

#####
Data summary
factor  x.mean      x.sd  x.median x.n
1  mud 12675.4779 7624.5690 9653.3553 26
2  silt 3470.0049  677.7561 3562.5775  8
3  sand  719.7101  572.6703  586.6125 30
```

4.6.4 H₂S



```
#####
Shapiro-Wilk normality test

data: resid(lm(data ~ factor))
W = 0.63318, p-value = 2.246e-11

=> Residuals are rejected to be normal distributed (Shapiro-Wilks's p-value < 0.05 )

#####
Kruskal-Wallis rank sum test

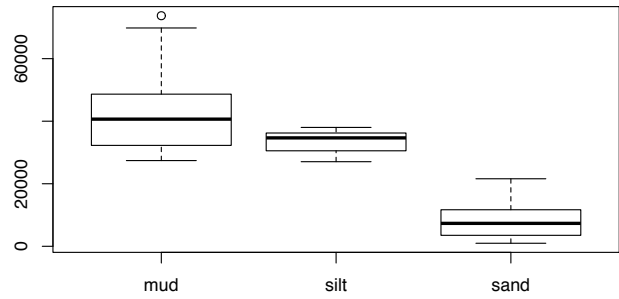
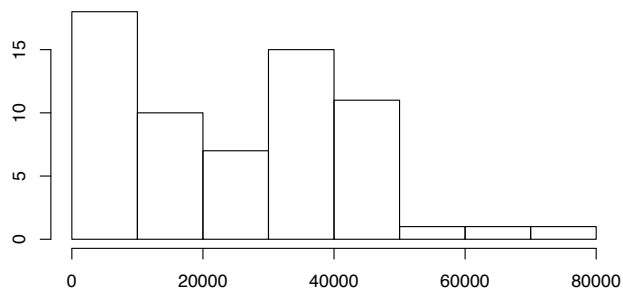
data: data and factor
Kruskal-Wallis chi-squared = 30.973, df = 2, p-value = 0

      Comparison of data by factor
      (No adjustment)
Col Mean-|
Row Mean |      mud      sand
-----|-----
sand |  4.672803
      |  0.0000*
      |
silt | -1.256055 -4.247625
      |  0.1045  0.0000*

alpha = 0.05
Reject Ho if p <= alpha/2
Table above shows Dunn's test z-statistic (upper line) and p-value (lower line)

#####
Data summary
factor  x.mean    x.sd  x.median x.n
1  mud 14855.1779 21511.080 5549.5682 26
2  silt 12057.1200 2038.479 12087.9000  7
3  sand  919.9535  1275.365  216.2125 31
```

4.6.5 H_4SiO_4



```
#####
Shapiro-Wilk normality test

data: resid(lm(data ~ factor))
W = 0.91403, p-value = 0.0002825

=> Residuals are rejected to be normal distributed (Shapiro-Wilks's p-value < 0.05 )

#####
Kruskal-Wallis rank sum test

data: data and factor
Kruskal-Wallis chi-squared = 48.3034, df = 2, p-value = 0

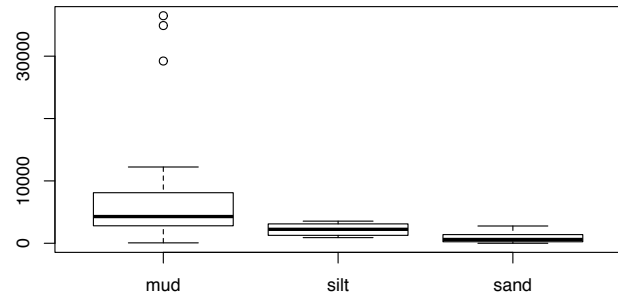
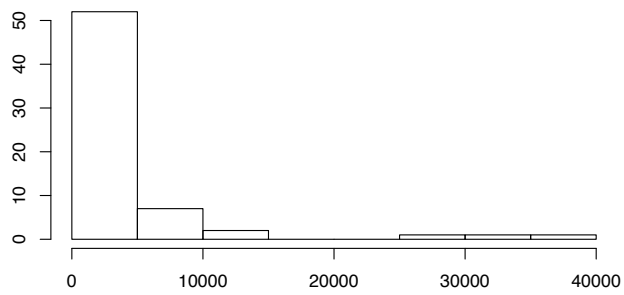
      Comparison of data by factor
      (No adjustment)

Col Mean-|
Row Mean |      mud      sand
-----|-----
sand | 6.807452
      | 0.0000*
      |
silt | 1.107444 -3.458769
      | 0.1341  0.0003*

alpha = 0.05
Reject Ho if p <= alpha/2
Table above shows Dunn's test z-statistic (upper line) and p-value (lower line)

#####
Data summary
factor  x.mean    x.sd  x.median x.n
1  mud 41975.898 11541.497 40658.703 26
2  silt 33489.711 4144.096 34665.762  8
3  sand 8418.926  5685.405  7329.893 30
```

4.6.6 Fe²⁺



```
#####
Shapiro-Wilk normality test

data: resid(lm(data ~ factor))
W = 0.59625, p-value = 5.439e-12

=> Residuals are rejected to be normal distributed (Shapiro-Wilks's p-value < 0.05 )

#####
Kruskal-Wallis rank sum test

data: data and factor
Kruskal-Wallis chi-squared = 28.4064, df = 2, p-value = 0

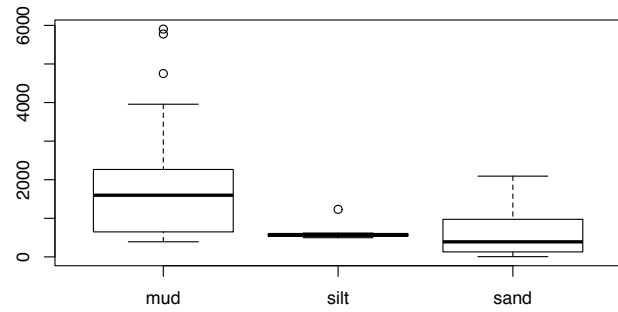
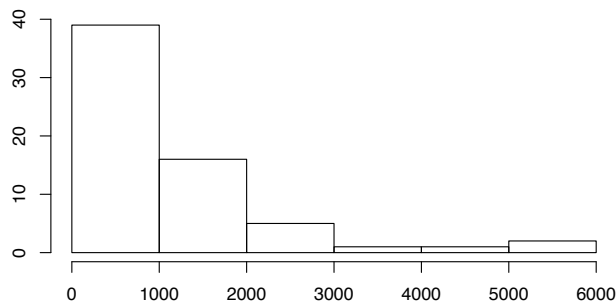
      Comparison of data by factor
      (No adjustment)

Col Mean-|
Row Mean |      mud      sand
-----|-----
sand |  5.294856
      |  0.0000*
      |
silt |  1.310539 -2.233859
      |  0.0950  0.0127*

alpha = 0.05
Reject Ho if p <= alpha/2
Table above shows Dunn's test z-statistic (upper line) and p-value (lower line)

#####
Data summary
factor  x.mean    x.sd  x.median x.n
1  mud 7898.9129 9978.2423 4285.4335 26
2  silt 2210.7223 1024.6186 2237.6401  8
3  sand 866.3453  786.5041  609.3959 30
```

4.6.7 Mn^{2+}



```
#####
Shapiro-Wilk normality test

data: resid(lm(data ~ factor))
W = 0.81122, p-value = 1.304e-07

=> Residuals are rejected to be normal distributed (Shapiro-Wilks's p-value < 0.05 )

#####
Kruskal-Wallis rank sum test

data: data and factor
Kruskal-Wallis chi-squared = 19.3943, df = 2, p-value = 0

Comparison of data by factor
(No adjustment)

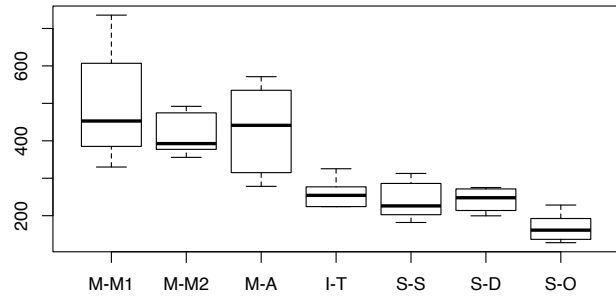
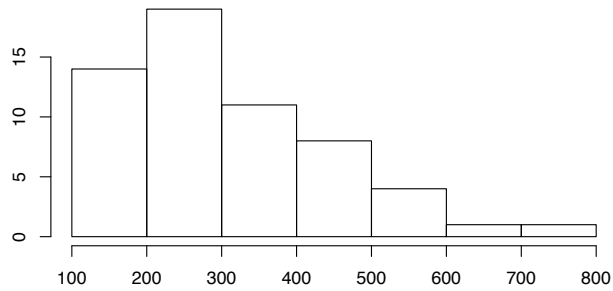
Col Mean-|
Row Mean |      mud      sand
-----|-----
sand | 4.385140
      | 0.0000*
      |
silt | 1.936431 -0.985327
      | 0.0264  0.1622

alpha = 0.05
Reject Ho if p <= alpha/2
Table above shows Dunn's test z-statistic (upper line) and p-value (lower line)

#####
Data summary
factor  x.mean  x.sd x.median x.n
1  mud 1854.4042 1585.1277 1598.312 26
2  silt 642.0250 241.5162 562.763 8
3  sand 573.0983 524.9071 389.750 30
```

4.7 Benthic solute reservoirs vs site

4.7.1 DIC



```
#####
Shapiro-Wilk normality test

data: resid(lm(data ~ factor))
W = 0.97166, p-value = 0.1918

=> Residuals are accepted as normal distributed (Shapiro-Wilks's p-value > 0.05 )

#####
Bartlett test of homogeneity of variances

data: data and factor
Bartlett's K-squared = 28.341, df = 6, p-value = 8.105e-05

=> Group variances are rejected to be equal (Bartlett's p-value < 0.05 )

#####
Kruskal-Wallis rank sum test

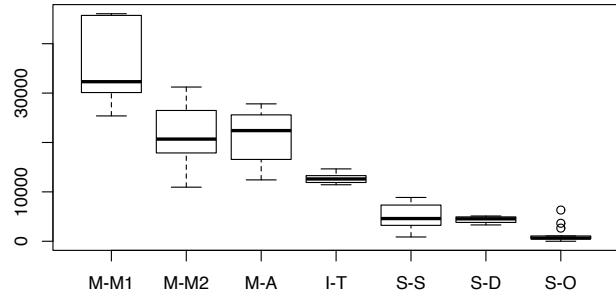
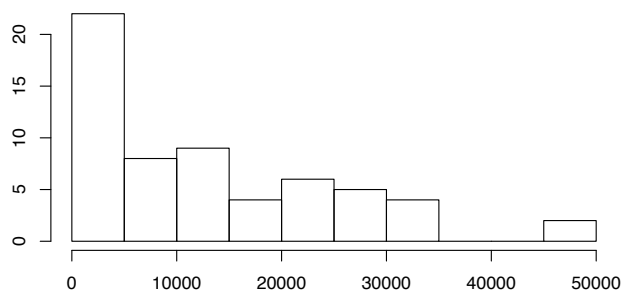
data: data and factor
Kruskal-Wallis chi-squared = 45.8761, df = 6, p-value = 0
```

Col Mean-						
Row Mean	I-T	M-A	M-M1	M-M2	S-D	S-O
M-A	-2.174990					
	0.0148*					
M-M1	-2.435441	-0.470357				
	0.0074*	0.3190				
M-M2	-2.085711	-0.075531	0.364010			
	0.0185*	0.4699	0.3579			
S-D	0.282863	2.207116	2.453068	2.142638		
	0.3886	0.0137*	0.0071*	0.0161*		
S-O	2.062745	5.031904	5.017563	4.608450	1.470139	
	0.0196*	0.0000*	0.0000*	0.0000*	0.0708	
S-S	0.523088	3.233972	3.398898	2.989785	0.136757	-1.885686
	0.3005	0.0006*	0.0003*	0.0014*	0.4456	0.0297

```
alpha = 0.05
Reject Ho if p <= alpha/2
Table above shows Dunn's test z-statistic (upper line) and p-value (lower line)
```

```
#####
Data summary
factor  x.mean  x.sd x.median x.n
1 M-M1 500.3523 150.81972 452.8613 7
2 M-M2 420.5394 57.44121 392.4900 7
3 M-A 429.8236 107.83847 441.2883 10
4 I-T 259.9203 38.77795 254.2988 6
5 S-S 240.6590 48.08814 226.1485 12
6 S-D 242.6681 35.34463 247.9318 4
7 S-O 169.4134 34.87701 161.3965 12
```


4.7.2 NH₄⁺



```
#####
Shapiro-Wilk normality test

data: resid(lm(data ~ factor))
W = 0.94682, p-value = 0.01107

=> Residuals are rejected to be normal distributed (Shapiro-Wilks's p-value < 0.05 )

#####
Kruskal-Wallis rank sum test

data: data and factor
Kruskal-Wallis chi-squared = 52.3319, df = 6, p-value = 0

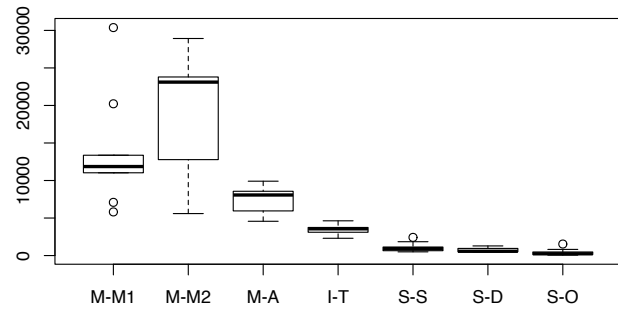
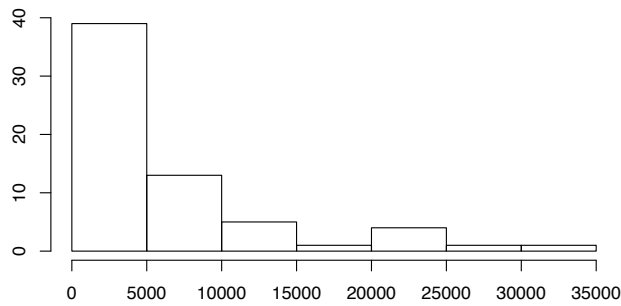
Comparison of data by factor
(No adjustment)

Col Mean |
Row Mean |      I-T      M-A      M-M1      M-M2      S-D      S-O
-----|-----
M-A | -1.188473
      0.1173
M-M1 | -2.136831 -1.167969
      0.0163*  0.1214
M-M2 | -1.086536  0.009959  1.092920
      0.1386  0.4960  0.1372
S-D |  1.422529  2.497099  3.223004  2.349130
      0.0774  0.0063*  0.0006*  0.0094*
S-O |  3.282999  5.051516  5.527155  4.521842  1.132403
      0.0005*  0.0000*  0.0000*  0.0000*  0.1287
S-S |  1.789140  3.386526  4.108181  3.027983 -0.092441 -1.785502
      0.0368  0.0004*  0.0000*  0.0012*  0.4632  0.0371

alpha = 0.05
Reject Ho if p <= alpha/2
Table above shows Dunn's test z-statistic (upper line) and p-value (lower line)

#####
Data summary
factor      x.mean      x.sd      x.median x.n
1 M-M1 35317.681 8652.3965 32308.359 6
2 M-M2 21654.731 7082.3721 20687.350 7
3 M-A 21345.547 5234.7171 22405.568 10
4 I-T 12727.192 1114.5501 12617.700 7
5 S-S 4957.739 2659.5530 4597.442 13
6 S-D 4375.534 782.6206 4541.825 4
7 S-O 1366.885 1816.1883 637.150 13
```

4.7.3 PO₄



```
#####
Shapiro-Wilk normality test

data: resid(lm(data ~ factor))
W = 0.75143, p-value = 4.599e-09

=> Residuals are rejected to be normal distributed (Shapiro-Wilks's p-value < 0.05 )

#####
Kruskal-Wallis rank sum test

data: data and factor
Kruskal-Wallis chi-squared = 56.6471, df = 6, p-value = 0
```

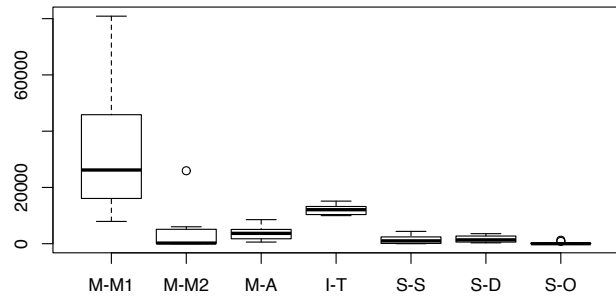
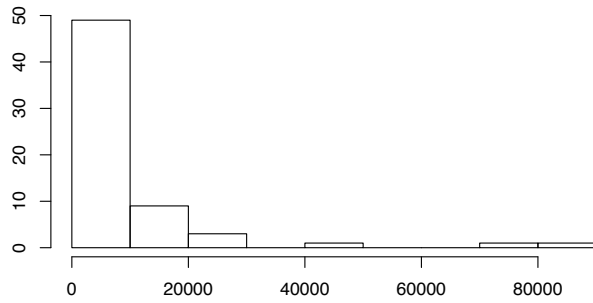
Comparison of data by factor
(No adjustment)

Col Mean-						
Row Mean	I-T	M-A	M-M1	M-M2	S-D	S-O
M-A	-1.302118 0.0964					
M-M1	-2.130800 0.0166*	-0.909167 0.1816				
M-M2	-2.260810 0.0119*	-1.120993 0.1311	-0.267282 0.3946			
S-D	1.512925 0.0651	2.610043 0.0045*	3.264726 0.0005*	3.344943 0.0004*		
S-O	3.075415 0.0011*	4.753940 0.0000*	5.574687 0.0000*	5.443697 0.0000*	0.796629 0.2128	
S-S	1.521617 0.0641	3.093990 0.0010*	3.964528 0.0000*	3.954359 0.0000*	-0.424507 0.3356	-1.780098 0.0375

```
alpha = 0.05
Reject Ho if p <= alpha/2
Table above shows Dunn's test z-statistic (upper line) and p-value (lower line)

#####
Data summary
factor  x.mean  x.sd  x.median x.n
1 M-M1 13683.1623 7463.7958 11860.8750 9
2 M-M2 18683.2107 8718.9520 23109.5438 7
3 M-A 7563.1491 1776.9105 8071.0767 10
4 I-T 3470.0049 677.7561 3562.5775 8
5 S-S 1058.8111 582.9742 928.6050 13
6 S-D 729.1735 374.1973 571.1265 4
7 S-O 377.6974 407.8748 241.7286 13
```

4.7.4 H₂S



```
#####
Shapiro-Wilk normality test

data: resid(lm(data ~ factor))
W = 0.64893, p-value = 4.237e-11

=> Residuals are rejected to be normal distributed (Shapiro-Wilks's p-value < 0.05 )

#####
Kruskal-Wallis rank sum test

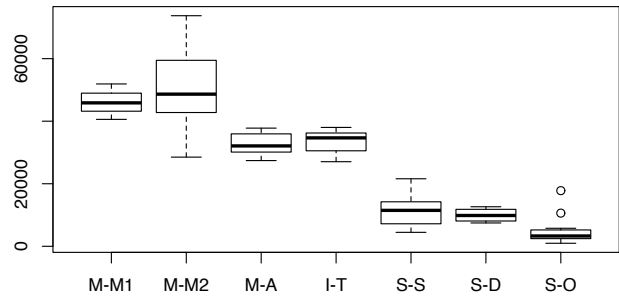
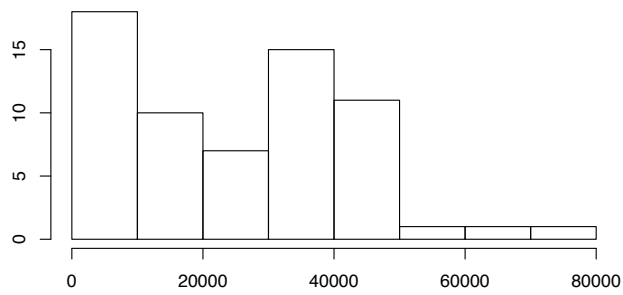
data: data and factor
Kruskal-Wallis chi-squared = 47.2572, df = 6, p-value = 0
```

Comparison of data by factor (No adjustment)						
Col Mean-	I-T	M-A	M-M1	M-M2	S-D	S-O
Row Mean						
M-A	1.610239 0.0537					
M-M1	-0.590525 0.2774	-2.374769 0.0088*				
M-M2	2.311560 0.0104*	0.896999 0.1849	3.042305 0.0012*			
S-D	1.998854 0.0228*	0.776382 0.2188	2.580096 0.0049*	0.027549 0.4890		
S-O	4.874118 0.0000*	3.532861 0.0002*	5.977520 0.0000*	2.204958 0.0137*	1.769884 0.0384	
S-S	3.036022 0.0012*	1.497244 0.0672	3.968612 0.0000*	0.400437 0.3444	0.298126 0.3828	-2.162633 0.0153*

```
alpha = 0.05
Reject Ho if p <= alpha/2
Table above shows Dunn's test z-statistic (upper line) and p-value (lower line)
```

```
#####
Data summary
factor  x.mean  x.sd  x.median x.n
1 M-M1 34317.5037 26807.7730 26200.11250 9
2 M-M2 5235.4069 9443.0674 215.64875 7
3 M-A 4072.9244 2676.9133 3679.89812 10
4 I-T 12057.1200 2038.4789 12087.90000 7
5 S-S 1493.5188 1489.9278 1010.40000 13
6 S-D 1652.0349 1436.3409 1366.37125 4
7 S-O 178.1911 376.7668 5.57625 14
```

4.7.5 H₄SiO₄



```
#####
Shapiro-Wilk normality test

data: resid(lm(data ~ factor))
W = 0.88887, p-value = 3.123e-05

=> Residuals are rejected to be normal distributed (Shapiro-Wilks's p-value < 0.05 )

#####
Kruskal-Wallis rank sum test

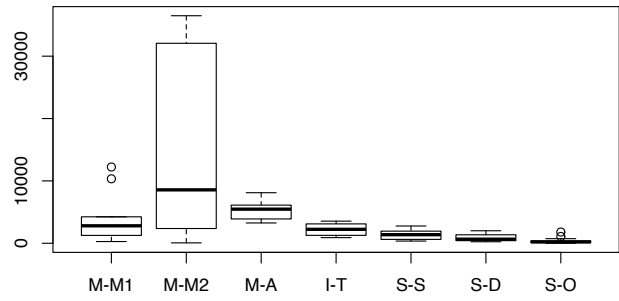
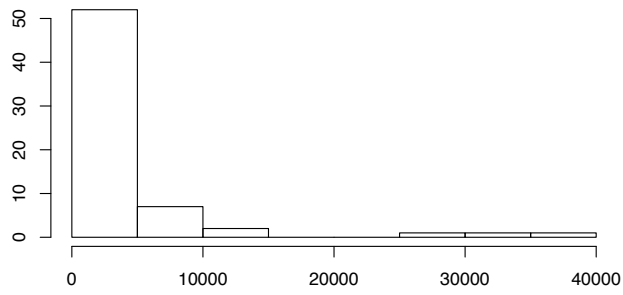
data: data and factor
Kruskal-Wallis chi-squared = 55.5131, df = 6, p-value = 0
```

Col Mean	I-T	M-A	M-M1	M-M2	S-D	S-O
Row Mean						
M-A	0.161349 0.4359					
M-M1	-1.631873 0.0514	-1.892367 0.0292				
M-M2	-1.454701 0.0729	-1.683046 0.0462	0.079508 0.4683			
S-D	1.874711 0.0304	1.811143 0.0351	3.229968 0.0006*	3.032789 0.0012*		
S-O	3.830477 0.0001*	3.910214 0.0000*	5.798056 0.0000*	5.277515 0.0000*	1.002561 0.1580	
S-S	2.451367 0.0071*	2.436885 0.0074*	4.368920 0.0000*	3.955618 0.0000*	-0.081288 0.4676	-1.579968 0.0571

```
alpha = 0.05
Reject Ho if p <= alpha/2
Table above shows Dunn's test z-statistic (upper line) and p-value (lower line)
```

```
#####
Data summary
factor    x.mean    x.sd    x.median x.n
1  M-M1 45630.885  3941.778 45865.500  9
2  M-M2 50769.132 16045.659 48648.259  7
3  M-A 32531.147  3457.093 32096.324 10
4  I-T 33489.711  4144.096 34665.762  8
5  S-S 11504.246  5546.436 11486.487 13
6  S-D 9951.768  2314.812 9851.387  4
7  S-O 4861.962  4605.582 3294.062 13
```

4.7.6 Fe²⁺



```
#####
Shapiro-Wilk normality test

data: resid(lm(data ~ factor))
W = 0.705, p-value = 4.813e-10

=> Residuals are rejected to be normal distributed (Shapiro-Wilks's p-value < 0.05 )

#####
Kruskal-Wallis rank sum test

data: data and factor
Kruskal-Wallis chi-squared = 35.6882, df = 6, p-value = 0
```

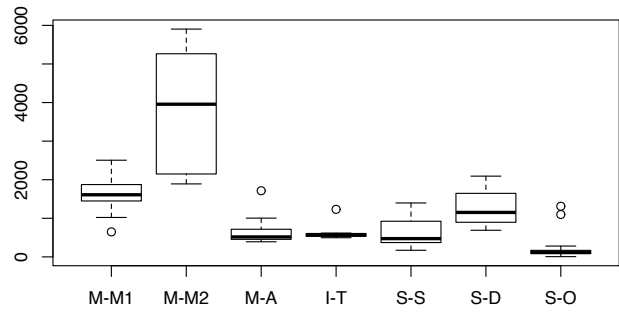
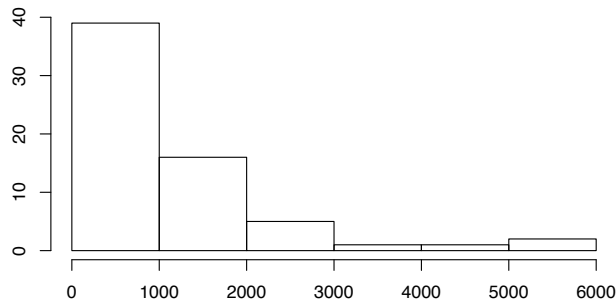
Comparison of data by factor
(No adjustment)

Col Mean-						
Row Mean	I-T	M-A	M-M1	M-M2	S-D	S-O
M-A	-1.851272 0.0321					
M-M1	-0.328523 0.3713	1.563768 0.0589				
M-M2	-0.982155 0.1630	0.750442 0.2265	-0.691889 0.2445			
S-D	1.315587 0.0942	2.846082 0.0022*	1.606295 0.0541	2.096327 0.0180*		
S-O	2.962787 0.0015*	5.252907 0.0000*	3.438394 0.0003*	3.924145 0.0000*	0.919465 0.1789	
S-S	1.050422 0.1468	3.209891 0.0007*	1.456659 0.0726	2.091114 0.0183*	-0.583472 0.2798	-2.190890 0.0142*

```
alpha = 0.05
Reject Ho if p <= alpha/2
Table above shows Dunn's test z-statistic (upper line) and p-value (lower line)
```

```
#####
Data summary
factor    x.mean    x.sd  x.median x.n
1 M-M1  4172.1413  4268.3985 2802.1620  9
2 M-M2 16282.8387 16531.6816 8566.3479  7
3 M-A   5384.2594  1610.1922 5468.8101 10
4 I-T   2210.7223  1024.6186 2237.6401  8
5 S-S   1317.5243   793.2899 1377.6987 13
6 S-D   889.7431   770.7439  654.5160  4
7 S-O   407.9671   518.4343  217.9714 13
```

4.7.7 Mn²⁺



```
#####
Shapiro-Wilk normality test

data: resid(lm(data ~ factor))
W = 0.86797, p-value = 6.041e-06

=> Residuals are rejected to be normal distributed (Shapiro-Wilks's p-value < 0.05 )

#####
Kruskal-Wallis rank sum test

data: data and factor
Kruskal-Wallis chi-squared = 42.3039, df = 6, p-value = 0

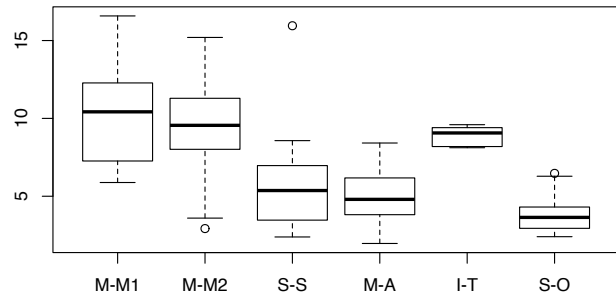
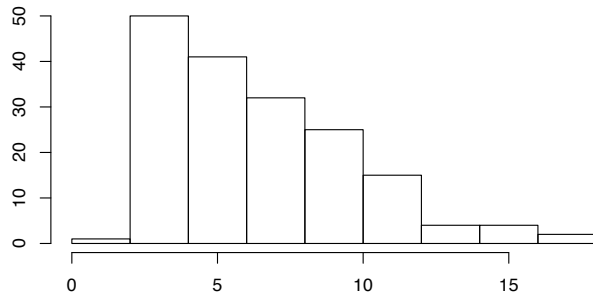
Comparison of data by factor
(No adjustment)

Col Mean-|
Row Mean |
-----|-----
M-A | 0.113227
      | 0.4549
M-M1 | -2.198347 -2.441764
      | 0.0140* 0.0073*
M-M2 | -3.113247 -3.378548 -1.077588
      | 0.0009* 0.0004* 0.1406
S-D | -1.271734 -1.407154 0.481640 1.328184
      | 0.1017 0.0797 0.3150 0.0921
S-O | 2.151411 2.170704 4.692858 5.499090 3.052843
      | 0.0157* 0.0150* 0.0000* 0.0000* 0.0011*
S-S | 0.395344 0.294665 2.873091 3.815875 1.672741 -2.011827
      | 0.3463 0.3841 0.0020* 0.0001* 0.0472 0.0221*

alpha = 0.05
Reject Ho if p <= alpha/2
Table above shows Dunn's test z-statistic (upper line) and p-value (lower line)

#####
Data summary
factor x.mean x.sd x.median x.n
1 M-M1 1634.0054 571.5146 1610.1250 9
2 M-M2 3796.9879 1750.7843 3956.7137 7
3 M-A 692.9545 404.0054 517.1149 10
4 I-T 642.0250 241.5162 562.7630 8
5 S-S 648.9829 379.3994 473.0080 13
6 S-D 1271.8611 590.4150 1152.3295 4
7 S-O 282.2098 417.2582 118.3477 13
```

4.8 ChIA in top 5 mm vs site



```
#####
Shapiro-Wilk normality test

data: resid(lm(data ~ factor))
W = 0.95762, p-value = 4.129e-05

=> Residuals are rejected to be normal distributed (Shapiro-Wilks's p-value < 0.05 )

#####
Kruskal-Wallis rank sum test

data: data and factor
Kruskal-Wallis chi-squared = 91.5398, df = 5, p-value = 0

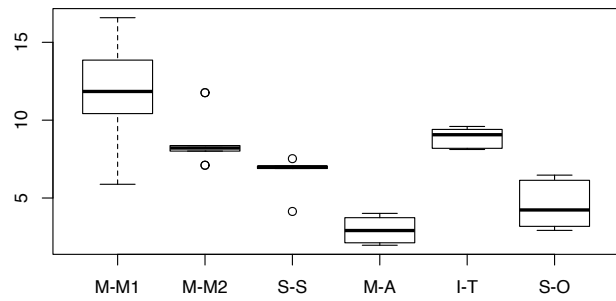
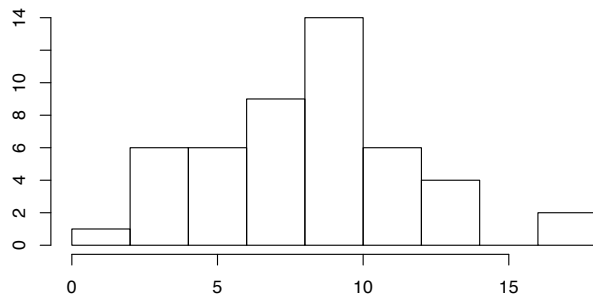
Comparison of data by factor
(No adjustment)

Col Mean-|
Row Mean |      I-T      M-A      M-M1      M-M2      S-O
-----|-----
M-A |      3.022198
      |      0.0013*
M-M1 |     -0.088909     -4.886518
      |      0.4646      0.0000*
M-M2 |      0.238869     -5.457740      0.510067
      |      0.4056      0.0000*      0.3050
S-O |      4.345931      2.756383      6.783708      7.683609
      |      0.0000*      0.0029*      0.0000*      0.0000*
S-S |      2.866300     -0.115158      4.440028      4.759245     -2.566788
      |      0.0021*      0.4542      0.0000*      0.0000*      0.0051*

alpha = 0.05
Reject Ho if p <= alpha/2
Table above shows Dunn's test z-statistic (upper line) and p-value (lower line)

#####
Data summary
factor      x.mean      x.sd x.median x.n
1 M-M1 10.325722 3.4570047 10.4220 18
2 M-M2  9.407417 3.0094876  9.5540 36
3 S-S  5.497200 2.6236764  5.3670 30
4 M-A  5.091375 1.7164939  4.8000 48
5 I-T  8.906833 0.6178956  9.0650  6
6 S-O  3.802972 1.1343805  3.6415 36
```

4.9 ChIA in top 5 mm vs site (EMB111 only)



```
#####
Shapiro-Wilk normality test

data: resid(lm(data ~ factor))
W = 0.89771, p-value = 0.0005309

=> Residuals are rejected to be normal distributed (Shapiro-Wilks's p-value < 0.05 )

#####
Kruskal-Wallis rank sum test

data: data and factor
Kruskal-Wallis chi-squared = 34.1382, df = 5, p-value = 0

Comparison of data by factor
(No adjustment)

Col Mean-|
Row Mean |
-----|-----
M-A | 3.382908
      | 0.0004*
M-M1 | -0.833650 -4.739896
      | 0.2022 0.0000*
M-M2 | 0.428734 -3.477511 1.546098
      | 0.3341 0.0003* 0.0610
S-O | 2.743456 -0.639452 4.001520 2.739136
      | 0.0030* 0.2613 0.0000* 0.0031*
S-S | 1.835846 -1.547061 2.953503 1.691118 -0.907609
      | 0.0332 0.0609 0.0016* 0.0454 0.1820

alpha = 0.05
Reject Ho if p <= alpha/2
Table above shows Dunn's test z-statistic (upper line) and p-value (lower line)

#####
Data summary
factor x.mean x.sd x.median x.n
1 M-M1 11.738167 3.4210377 11.8435 12
2 M-M2 8.612500 1.5346824 8.2110 12
3 S-S 6.602833 1.2284106 7.0065 6
4 M-A 2.944000 0.9157720 2.9115 6
5 I-T 8.906833 0.6178956 9.0650 6
6 S-O 4.529167 1.4809990 4.2335 6
```