Mass Discharge - Outlet Alteck. 2016

PAZ

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Purpose

This file merges "sub-weekly" (i.e. sample) outlet concentrations (S-met and TPs) and $\delta^{13}C$ in dissolved and sediment samples. Hydrochemistry variables are also merged.

To do that it imports lab results for isotopes (^{13}C) and s-metolachlor concentrations, as well as the weekly discharge summary (*WeeklyHydro_R.csv*).

Imports:

- **WeeklyHydro_R.csv** (R generated, Book 3)
- **fluxAlteck2016_R.csv** (R generated, Book 4)
- **OutletConc_W0toW17.csv**
- **MESAlteckWater.csv** (Concentration in filters)
- **Outlet_Isotopes_W0toW17.csv**
- **MESAlteck_FilterIsotopes.csv** (Isotopes in filters)
- **Outlet_ESAOXA_W0toW17.csv**
- **AO-Hydrochem.csv**

Generates:

- **WeeklyHydroContam_R.csv**

Required R-packages:

```
library("stringr")
library("plyr")
library("dplyr")
library("zoo")
library("ggplot2")
library("plotly")
```

Working directory

```
# setwd("D:/Documents/these_pablo/Alteckendorf2016/R")
# setwd("/Users/DayTightChunks/Documents/PhD/Routput/Alteck/R")
# setwd("D:/Documents/these_pablo/Alteckendorf2016/00_TransparencyFolder")
getwd()
```

```
## [1] "/Users/DayTightChunks/Documents/PhD/HydrologicalMonitoring"
```

Lab and reference values

```
source("global.R")
```

Outlet Data - Alteckendorf 2016

Hydrological data on a subweekly basis

```
weeklyhydro = read.csv2("Data/WeeklyHydro_R.csv", header = TRUE)
colnames(weeklyhydro)[colnames(weeklyhydro) == "ID"] <- "WeekSubWeek"
head(weeklyhydro)
```

```
##   WeekSubWeek AveDischarge.m3.h Volume.m3 Sampled.Hrs     Sampled
## 1       W0-0x          1.204775  14.41714    11.96667 Not Sampled
## 2        W0-1          1.213511 100.15508    82.53333     Sampled
## 3       W0-2x          1.284719  48.34827    37.63333 Not Sampled
## 4        W1-1         14.316647 390.36726    27.26667     Sampled
## 5        W1-2         15.529299 359.24445    23.13333     Sampled
## 6       W1-3x          9.107720 877.37700    96.33333 Not Sampled
##   CumRain.mm RainInt.mmhr
## 1        2.8   0.23398329
## 2        7.6   0.09208401
## 3        7.6   0.20194863
## 4       16.8   0.61613692
## 5        6.0   0.25936599
## 6        9.4   0.09757785
```

```
weeklyflux = read.csv2("Data/fluxAlteck2016_R.csv", header = TRUE)
head(weeklyflux)
```

```
##   WeekSubWeek                  ti                  tf     iflux     fflux
## 1       W0-0x 2016-03-25 00:04:00 2016-03-25 12:02:00  1.248600  1.129227
## 2        W0-1 2016-03-25 12:04:00 2016-03-28 22:36:00  1.124382  1.313125
## 3       W0-2x 2016-03-28 22:38:00 2016-03-30 12:16:00  1.308100  1.456349
## 4        W1-1 2016-03-30 12:18:00 2016-03-31 15:34:00  1.456080 16.445436
## 5        W1-2 2016-03-31 15:36:00 2016-04-01 14:44:00 16.334349 15.184536
## 6       W1-3x 2016-04-01 14:46:00 2016-04-05 15:06:00 15.203629  5.856380
##   changeflux      maxQ      minQ  dryHrsIni dryHrsMax dryHrsAve
## 1 -0.1193728  1.248600  1.118296 0.01666667  2.750000 0.7449537
## 2  0.1887431  1.380388  1.082199 0.03333333 24.516667 7.8272574
## 3  0.1482496  1.637782  0.929055 0.26666667 13.316667 4.8591888
## 4 14.9893566 38.399790  1.448977 0.11666667  4.200000 1.2885633
## 5 -1.1498131 18.668972 13.201113 4.21666667  5.433333 1.3142446
## 6 -9.3472489 15.895640  5.471042 3.41666667 29.716667 9.4699181
##   noEventHrsIni noEventHrsMax noEventHrsAve Duration.Hrs  chExtreme Event
## 1    0.01666667      6.000000      3.008333     11.96667 -0.1303036    NA
## 2    6.01666667     47.283333     26.650000     82.53333  0.2560062    NA
## 3   47.30000000     66.116667     56.708333     37.63333  0.3296817    NA
## 4   66.13333333     72.100000     30.395503     27.26667 36.9437102     1
## 5    1.65000000      6.366667      3.329089     23.13333 -3.1332355    NA
## 6    6.26666667     54.433333     30.350000     96.33333 -9.7325862    NA
##    Markers TimeDiff
## 1       NA     <NA>
```

```
## 2       NA     <NA>
## 3       NA     <NA>
## 4 16.88972       24
## 5       NA     <NA>
## 6       NA     <NA>
```

Concentration data (dissolved and suspended solids) on a subweekly basis

```
outletConc = read.csv2("Data/OutletConc_W0toW17.csv", sep = ",", dec =".", header = T)
outletConc$ID4 <- as.character(outletConc$ID4)
outletConc <- outletConc[outletConc$ID4 != "J+7", ]
outletConc$Vol.SPE.L <- outletConc$Vol.SPE.mL/1000
outletConc <- outletConc[,c("WeekSubWeek", "Conc.mug.L", "Conc.SD", "Vol.SPE.L", "Conc.in500uL")]
head(outletConc)
```

```
##   WeekSubWeek Conc.mug.L Conc.SD Vol.SPE.L Conc.in500uL
## 1        W0-1  0.2456594 0.01931     0.570     140.0258
## 2        W1-1  6.7882463 0.28942     1.910   12965.5505
## 3        W1-2  6.5609982 0.19064     1.910   12531.5066
## 4        W2-1  9.4443019 0.33354     1.800   16999.7434
## 5        W2-2  1.0421883 0.03904     2.025    2110.4313
## 6        W3-1  8.8357358 0.47086     1.180   10426.1682
```

```
filters = read.csv2("Data/MESAlteckWater.csv")
filters$MO.mg.L = ifelse(filters$MO.mg.L < 0, 0.0001, filters$MO.mg.L)
head(filters)
```

```
##   WeekSubWeek  MES.mg.L MES.sd MO.mg.L Conc.Solids.mug.gMES
## 1        W0-1  53.44444     NA  0.0000           0.64472899
## 2        W1-1  62.50000     NA  0.0010           0.12588974
## 3        W1-2  22.50000     NA  0.0001           0.43578716
## 4        W2-1  22.50000     NA  0.0001           0.07935267
## 5        W2-2   5.00000     NA  0.0001           0.05075270
## 6        W3-1 197.50000     NA  0.0058           0.08177487
##   Conc.Solids.ug.gMES.SD
## 1            0.023237548
## 2            0.027063685
## 3            0.123237064
## 4            0.004683719
## 5            0.001027205
## 6            0.001343089
```

```
# MESA/MOXA data cleaning
outletESAOXA = read.csv2("Data/Outlet_ESAOXA_W0toW17.csv", header = T)
outletESAOXA$ID <- as.character(outletESAOXA$ID)
split <- strsplit(outletESAOXA$ID, "-", fixed = TRUE)
outletESAOXA$ESAOXA_SD <- sapply(split, "[", 4)
split_vor <- strsplit(outletESAOXA$ID, "-SD", fixed = TRUE)
outletESAOXA$ESAOXA_Mean <- sapply(split_vor, "[", 1)

means_temp <- subset(outletESAOXA, is.na(outletESAOXA$ESAOXA_SD))
sd_temp <- subset(outletESAOXA, !is.na(outletESAOXA$ESAOXA_SD))
means_temp$ID <- NULL
sd_temp$ID <- NULL
```

```r
head(sd_temp)
```

```
##       MOXA.ugL    MESA.ugL ESAOXA_SD ESAOXA_Mean
## 2  1.141445314 3.497220592        SD     AO-W0-1
## 4  10.18525095 3.036984548        SD     AO-W1-1
## 6  0.243054437 0.853382023        SD     AO-W1-2
## 8  1.152648881  2.82619239        SD     AO-W2-1
## 10 0.610001114 0.191041941        SD     AO-W2-2
## 12 2.658942145 0.326863705        SD     AO-W3-1
```

```r
head(means_temp)
```

```
##       MOXA.ugL    MESA.ugL ESAOXA_SD ESAOXA_Mean
## 1  4.824094386 18.05530754      <NA>     AO-W0-1
## 3  30.53123497 45.98364257      <NA>     AO-W1-1
## 5  32.49246534 41.28051586      <NA>     AO-W1-2
## 7  104.5412549 98.56782406      <NA>     AO-W2-1
## 9  26.88584879 51.95245249      <NA>     AO-W2-2
## 11 45.08067271 24.04717483      <NA>     AO-W3-1
```

```r
outletESAOXA <- merge(means_temp, sd_temp, by = "ESAOXA_Mean", all = T)
outletESAOXA$ESAOXA_SD.x <- NULL
outletESAOXA$ESAOXA_SD.y <- NULL
split_ID <- strsplit(outletESAOXA$ESAOXA_Mean, "AO-", fixed = T)
outletESAOXA$ID <- sapply(split_ID, "[", 2)
outletESAOXA$ESAOXA_Mean <- NULL
outletESAOXA <- outletESAOXA[ , c("ID", "MOXA.ugL.x", "MOXA.ugL.y", "MESA.ugL.x", "MESA.ugL.y")]
colnames(outletESAOXA) <- c("WeekSubWeek", "OXA_mean", "OXA_SD", "ESA_mean",  "ESA_SD")
outletESAOXA$WeekSubWeek <- as.factor(outletESAOXA$WeekSubWeek)

head(outletESAOXA)
```

```
##   WeekSubWeek    OXA_mean      OXA_SD    ESA_mean      ESA_SD
## 1        W0-1 4.824094386 1.141445314 18.05530754 3.497220592
## 2        W1-1 30.53123497 10.18525095 45.98364257 3.036984548
## 3        W1-2 32.49246534 0.243054437 41.28051586 0.853382023
## 4       W10-1 21.31142261 0.051684365 82.87549054 1.816721799
## 5       W10-2 13.09504645 0.177035158 12.02386661 0.305752134
## 6       W10-3 45.60580848 1.926635623 11.31491554 0.176347928
```

Isotope data

```r
# Outlet isotope data:

outletIso = read.csv2("Data/Outlet_Isotopes_W0toW17.csv", header = T, dec = ".")
if (length(outletIso) == 1){
  outletIso = read.csv("Data/Outlet_Isotopes_W0toW17.csv", header = T)
}
str(outletIso)
```

```
## 'data.frame':    106 obs. of  8 variables:
##  $ FileHeader..Filename: Factor w/ 103 levels "AO_W1_1-1_-0001.dxf",..: 1 2 3 4 5 6 40 41 42 52 ...
##  $ ID                  : Factor w/ 1 level "AO": 1 1 1 1 1 1 1 1 1 1 ...
##  $ Week                : Factor w/ 10 levels "W1","W10","W11",..: 1 1 1 1 1 1 5 5 5 6 ...
```

```
##  $ Wnum               : int  1 1 1 1 1 1 2 2 2 3 ...
##  $ SubWeek            : int  1 1 1 2 2 2 1 1 1 2 ...
##  $ WeekSubWeek        : Factor w/ 27 levels "W1-1","W1-2",..: 1 1 1 2 2 2 13 13 13 16 ...
##  $ Repl               : Factor w/ 7 levels "1","1b","2","3",..: 1 3 4 1 3 4 1 3 4 1 ...
##  $ d.13C.12C          : num  -31.6 -31.4 -31.4 -31.5 -31.8 ...
```

```
colnames(outletIso)
```

```
## [1] "FileHeader..Filename" "ID"                   "Week"
## [4] "Wnum"                 "SubWeek"              "WeekSubWeek"
## [7] "Repl"                 "d.13C.12C"
```

```
# Correct for extraction shift
outletIso$d.13C.12C = round( (outletIso$d.13C.12C - meanshift_w), 1)
outletIso$DD13 <- outletIso$d.13C.12C - initialDelta

# Filter isotope data:
filtersIso = read.csv2("Data/MESAlteck_FilterIsotopes.csv", header = T, dec = ".")
#filtersIso <- filtersIso[filtersIso$Levl != "J+7", ]
if (length(filtersIso) == 1){
  filtersIso = read.csv("Data/MESAlteck_FilterIsotopes.csv", header = T)
}
colnames(filtersIso)
```

```
## [1] "ID"           "Week"         "Wnum"         "Num"
## [5] "Levl"         "Repl"         "d.13C.12C"    "DD13.32.253."
## [9] "ng..C."
```

```
filtersIso$WeekSubWeek = paste(filtersIso$Week, filtersIso$Num, sep = "-")
colnames(filtersIso)[colnames(filtersIso) == "DD13.32.253."] <- "DD13"
colnames(filtersIso)[colnames(filtersIso) == "ng..C."] <- "ngC"

str(filtersIso)
```

```
## 'data.frame':    23 obs. of  10 variables:
##  $ ID         : Factor w/ 1 level "AFP": 1 1 1 1 1 1 1 1 1 1 ...
##  $ Week       : Factor w/ 3 levels "W2","W6","W9": 1 1 1 1 1 1 2 2 2 2 ...
##  $ Wnum       : int  1 1 1 2 2 2 3 3 3 3 ...
##  $ Num        : int  1 1 1 2 2 2 3 3 3 3 ...
##  $ Levl       : Factor w/ 2 levels "","J+7": 1 1 1 1 1 1 1 1 1 2 ...
##  $ Repl       : int  1 2 3 1 2 3 1 2 3 1 ...
##  $ d.13C.12C  : num  -26.2 -29.2 -29.3 -31.7 -27.4 ...
##  $ DD13       : num  6.056 3.023 2.927 0.592 4.906 ...
##  $ ngC        : num  0.73 0.83 0.83 0.664 0.73 ...
##  $ WeekSubWeek: chr  "W2-1" "W2-1" "W2-1" "W2-2" ...
```

Hydrochemistry Data

```
hydroChem = read.csv2("Data/AO-Hydrochem.csv", header = T)
hydroChem = hydroChem[, c("WeekSubWeek",
                          "NH4.mM",
                          "TIC.ppm.filt",
                          "Cl.mM",
                          "NO3...mM",
                          "PO4..mM",
```

```
                          "NPOC.ppm" ,
                          "TIC.ppm.unfilt",
                          "TOC.ppm.unfilt" )]
head(hydroChem)
```

```
##   WeekSubWeek NH4.mM TIC.ppm.filt   Cl.mM NO3...mM PO4..mM NPOC.ppm
## 1        W1-1   0.05         51.8    1.48   616.00      NA      4.0
## 2        W1-2     NA         44.8 1574.00   778.00      NA      4.4
## 3       W10-1     NA         60.1    1.17   964.00      NA      2.0
## 4       W10-2   9.00         57.1 1013.00  1174.00      13      5.2
## 5       W10-3     NA         58.2  858.00     1.23      NA      5.0
## 6       W10-4  15.00         26.4  355.00  1409.00      NA      6.4
##   TIC.ppm.unfilt TOC.ppm.unfilt
## 1           44.8            4.7
## 2           26.4            5.4
## 3           63.2            2.0
## 4           55.9            4.0
## 5           60.4            4.3
## 6           24.5            6.4
```

Summarizing IRMS data

```
outletIso <- outletIso[complete.cases(outletIso[ , "d.13C.12C"]), ]
isoOutSummary = ddply(outletIso, c("WeekSubWeek"), summarise,
                          N    = length(d.13C.12C),
                          diss.d13C = mean(d.13C.12C),
                          SD.d13C = sd(d.13C.12C),
                          # se.d13C = SD.d13C / sqrt(N),
                          N_d13C.diss = length(d.13C.12C))


isoFiltSummary = ddply(filtersIso, c("WeekSubWeek"), summarise,
                          N    = length(d.13C.12C),
                          filt.d13C = mean(d.13C.12C),
                          filt.SD.d13C = sd(d.13C.12C) #,
                          # filt.se.d13C = filt.SD.d13C / sqrt(N),
                          # N_ngC.fl = length(ngC),
                          # ngC.mean.fl = mean(ngC),
                          # ngC.SD.fl = sd(ngC)
                        )
head(isoFiltSummary)
```

```
##   WeekSubWeek N filt.d13C filt.SD.d13C
## 1        W2-1 3 -28.25333     1.778942
## 2        W2-2 3 -28.69333     2.573020
## 3        W6-3 6 -29.90667     1.617698
## 4        W9-1 2 -27.83500     1.746554
## 5        W9-2 3 -28.74000     2.011194
## 6        W9-3 3 -27.99000     1.685111
```

Merging and data wrangling stepts

Merge all data sets by the *WeekSubWeek* column ID, icluding:

```
# Dissolved
out.CoIs = merge(outletConc,  outletESAOXA, by = "WeekSubWeek", all = T)
out.CoIs = merge(out.CoIs, isoOutSummary, by = "WeekSubWeek", all = T)

# Filters (MES, Conc.MES)
out.CoIs = merge(out.CoIs, filters, by = "WeekSubWeek", all = T)
out.CoIs = merge(out.CoIs, isoFiltSummary, by= "WeekSubWeek", all = T)

# Remaining fraction
out.CoIs$DD13C.diss <- (out.CoIs$diss.d13C - (d13Co))
out.CoIs$DD13C.filt <- (out.CoIs$filt.d13C - (d13Co))


# Discharge times
out.CoIs = merge(weeklyhydro, out.CoIs, by = "WeekSubWeek", all = T)

# Discharge summary
out.CoIs = merge(weeklyflux, out.CoIs, by = "WeekSubWeek", all = T)




out.CoIs$tf <- as.POSIXct(out.CoIs$tf, "%Y-%m-%d %H:%M", tz = "EST")
out.CoIs$ti <- as.POSIXct(out.CoIs$ti, "%Y-%m-%d %H:%M", tz = "EST")
class(out.CoIs$tf)
```

```
## [1] "POSIXct" "POSIXt"
```

```
sum(is.na(out.CoIs$tf))
```

```
## [1] 5
```

```
write.csv(out.CoIs, "Data/MarkerResponse_R05.csv", row.names = F)

# Temprarily remove Weeks 16 & 17 (need to get discharge data)
# No discharge data yet avaialble to multiply against...
out.CoIs <- out.CoIs[!is.na(out.CoIs$tf), ]
```

Weekly Exported Solids (Kg)

```
# V[m3] * MES [mg/L] * 1000 [L/m3] * [1 Kg/10^6 mg]
out.CoIs$ExpMES.Kg = out.CoIs$Volume.m3*out.CoIs$MES.mg.L/1000
```

Weekly exported S-metolachlor mass (mg) - Linear interpolation

This section imputs concentrations missed due to sampler capacity being maxed out. For these subsets a linear interpolation value based on the trailing and leading observed concentrations was assumed. An approximative model will be tested at a later stage.

To revise: SD for filtered samples!! Note: Model may need to be improved!!!

```
# Assume first index is equivalent to second for all measured values
# (i.e. needed for na.approx operation below)
out.CoIs[1, c("Conc.mug.L")] <- out.CoIs[2, c("Conc.mug.L")]
out.CoIs[1, c("Conc.SD")] <- out.CoIs[2, c("Conc.SD")]
out.CoIs[1, c("Vol.SPE.L")] <- out.CoIs[2, c("Vol.SPE.L")]

out.CoIs[1, c("OXA_mean")] <- out.CoIs[2, c("OXA_mean")]
out.CoIs[1, c("OXA_SD")] <- out.CoIs[2, c("OXA_SD")]

out.CoIs[1, c("ESA_mean")] <- out.CoIs[2, c("ESA_mean")]
out.CoIs[1, c("ESA_SD")] <- out.CoIs[2, c("ESA_SD")]

out.CoIs[1, c("Conc.Solids.mug.gMES")] <- out.CoIs[2, c("Conc.Solids.mug.gMES")]
out.CoIs[1, c("Conc.Solids.ug.gMES.SD")] <- out.CoIs[2, c("Conc.Solids.ug.gMES.SD")]

out.CoIs[1, c("ExpMES.Kg")] <- out.CoIs[2, c("ExpMES.Kg")]

# Assign linear approximation of trailing and leading observed values
out.CoIs <- out.CoIs[with(out.CoIs , order(ti)), ]

val = out.CoIs$Volume.m3[nrow(out.CoIs)]
if (is.na(val)){
  out.CoIs = out.CoIs[1:nrow(out.CoIs)-1, ]
}


out.CoIs$Conc.mug.L <- na.approx(out.CoIs$Conc.mug.L)
out.CoIs$Conc.SD <- na.approx(out.CoIs$Conc.SD)

out.CoIs$OXA_mean <- na.approx(out.CoIs$OXA_mean)
out.CoIs$OXA_SD <- na.approx(out.CoIs$OXA_SD)

out.CoIs$ESA_mean <- na.approx(out.CoIs$ESA_mean)
out.CoIs$ESA_SD <- na.approx(out.CoIs$ESA_SD)

out.CoIs$Conc.Solids.mug.gMES <- na.approx(out.CoIs$Conc.Solids.mug.gMES)
out.CoIs$Conc.Solids.ug.gMES.SD <- na.approx(out.CoIs$Conc.Solids.ug.gMES.SD)

out.CoIs$ExpMES.Kg <- na.approx(out.CoIs$ExpMES.Kg)
```

Conversion of concentration to loadings (mass)

Exported mass observed at the outlet M for sample s is computed as,

$$M_s = C_s \cdot V_s$$

and,

$$V_s = \int_t^{\Delta t} Q(t)dt$$

where dt should be 2 min and Δt the length of the subsample.

Doubts with different expression:

$$V_s = \sum_{j=1}^{J} \int_0^2 Q(t)dt$$

where C the concentration $[\mu g/L]$ of sub-sample s, V is volume $[m^3]$, J is the array length of the 2-min interval composite sub-sample and Q is discharge.

```
# Dissolved - [mg] S-metolachlor exported per sub-week
# Conc. [mu.g s-meto/L H20] * Vol[m3] * [10^3 L/m^3] * [1 mg/10^3 mu.g]
out.CoIs$DissSmeto.mg = out.CoIs$Conc.mug.L*out.CoIs$Volume.m3
out.CoIs$DissSmeto.mg.SD = out.CoIs$Conc.SD*out.CoIs$Volume.m3
out.CoIs$DissSmeto.g = out.CoIs$DissSmeto.mg/10^3
out.CoIs$DissSmeto.g.SD = out.CoIs$DissSmeto.mg.SD/10^3

out.CoIs$DissOXA.mg = out.CoIs$OXA_mean*out.CoIs$Volume.m3
out.CoIs$DissOXA.mg.SD = out.CoIs$OXA_SD*out.CoIs$Volume.m3
out.CoIs$DissOXA.g = out.CoIs$DissOXA.mg/10^3
out.CoIs$DissOXA.g.SD = out.CoIs$DissOXA.mg.SD/10^3

out.CoIs$DissESA.mg = out.CoIs$ESA_mean*out.CoIs$Volume.m3
out.CoIs$DissESA.mg.SD = out.CoIs$ESA_SD*out.CoIs$Volume.m3
out.CoIs$DissESA.g = out.CoIs$DissESA.mg/10^3
out.CoIs$DissESA.g.SD = out.CoIs$DissESA.mg.SD/10^3

# Solids - [mg] S-metolachlor in solids exported per sub-week
# Conc. [mu.g s-meto / g MES] * Kg MES * [10^3 g/Kg] * [1 mg/10^3 mu.g]
out.CoIs$FiltSmeto.mg = out.CoIs$Conc.Solids.mug.gMES*out.CoIs$ExpMES.Kg
out.CoIs$FiltSmeto.mg.SD = out.CoIs$Conc.Solids.ug.gMES.SD*out.CoIs$ExpMES.Kg
out.CoIs$FiltSmeto.g = out.CoIs$FiltSmeto.mg/10^3
out.CoIs$FiltSmeto.g.SD  = out.CoIs$FiltSmeto.mg.SD/10^3

# Total SM
out.CoIs$TotSMout.mg = out.CoIs$DissSmeto.mg + out.CoIs$FiltSmeto.mg
out.CoIs$TotSMout.mg.SD = sqrt(((out.CoIs$DissSmeto.mg.SD)^2 + (out.CoIs$FiltSmeto.mg.SD)^2)/2)
out.CoIs$TotSMout.g = out.CoIs$TotSMout.mg/10^3
out.CoIs$TotSMout.g.SD = out.CoIs$TotSMout.mg.SD/10^3

# Distribution dissolved vs suspended solids
out.CoIs$FracDiss = out.CoIs$DissSmeto.mg/out.CoIs$TotSMout.mg
out.CoIs$FracFilt = out.CoIs$FiltSmeto.mg/out.CoIs$TotSMout.mg

#out.CoIs$DissSmeto.g = ifelse(is.na(out.CoIs$DissSmeto.g), 0.0, out.CoIs$DissSmeto.g)
#out.CoIs$FiltSmeto.g = ifelse(is.na(out.CoIs$FiltSmeto.g), 0.0, out.CoIs$FiltSmeto.g)
#out.CoIs$TotSMout.g = out.CoIs$DissSmeto.g + out.CoIs$FiltSmeto.g

write.csv2(out.CoIs,
           'Data/MonitoringScope_R.csv', row.names = F)
```

Molar mass equivalent exports

Mass equivalent loads are calculated such that:

$$MEQ_{SMET} = SMET_{out} + OXA_{out} * (\frac{mw_{SMET}}{mw_{MOXA}}) + ESA_{out} * (\frac{mw_{SMET}}{mw_{MESA}})$$

```
# Need to update this :
# out.CoIs$TotSMout.g.SD = out.CoIs$DissSmeto.g.SD

mw.SM <- 283.796 # g/mol
mw.MOXA <- 279.33 # g/ml
mw.MESA <- 329.1 # g/mol
out.CoIs$MELsm.g <-
  out.CoIs$TotSMout.g +
  out.CoIs$DissOXA.g * (mw.SM/mw.MOXA) +
  out.CoIs$DissESA.g * (mw.SM/mw.MESA)

# How to sum a standard deviation
# http://stats.stackexchange.com/questions/25848/how-to-sum-a-standard-deviation
out.CoIs$MELsm.g.SD <-
  sqrt((out.CoIs$TotSMout.g.SD^2 +
     (out.CoIs$DissOXA.g.SD * (mw.SM/mw.MOXA))^2 +
     (out.CoIs$DissESA.g.SD * (mw.SM/mw.MESA))^2)/3)

# Cumulative OUT
out.CoIs$CumOutDiss.g = cumsum(out.CoIs$DissSmeto.g)
out.CoIs$CumOutFilt.g = cumsum(out.CoIs$FiltSmeto.g)
out.CoIs$CumOutSmeto.g = out.CoIs$CumOutDiss.g + out.CoIs$CumOutFilt.g
out.CoIs$CumOutMELsm.g = cumsum(out.CoIs$MELsm.g)
```

Hydrochemistry

```
# Hydrochemistrty
# out.CoIs = merge(out.CoIs, hydroChem, by= "WeekSubWeek", all = F)
```

Application dates and masses

- **IMPORTANT: This is reviewed and final in Open Rayleigh - Revised (Book 09.3)**

Add the application dates and merge the total mass to the nearest discharge event

The 4 application dates were:

- 2016-03-20 (Friess, Beet) and 2016-03-25 (Matthis, Beet)
- 2016-04-13 and 2016-04-14 (Kopp and Burger, Beet)
- 2016-05-25 (Schmidt, Talweg, Corn)
- 2016-06-04 (Assumed Speich and Mahler, Corn not on transect, Except Speich N1)

So the total applied mass mass is merged at the nearest sampling time marker available :

```
ti = c(as.POSIXct('2016-03-25 00:04:00' , tz="EST"),
#       as.POSIXct('2016-04-05 15:08:00' , tz="EST"),
       as.POSIXct('2016-04-14 13:52:00' , tz="EST"),
       as.POSIXct('2016-05-29 12:10:00' , tz="EST"),
       # as.POSIXct('2016-05-24 12:00:00' , tz="EST"),
       as.POSIXct('2016-06-04 15:32:00' , tz="EST"))
```

```
# Appl.Mass.g = c(17319.059, 4744.571, 1891.742, 6826.825) # With Friess applying MG's doses for Beet
# Appl.Mass.g = c(33242.550, 4744.571, 1891.742, 6826.825) # With Friess applying DG's doses instead of
# Appl.Mass.g = c(31670.073, 4744.571, 1803.066, 6506.818) # With Friess applying MG's doses for Corn
Appl.Mass.g = c(31670.073, 12316.197, 1803.066, 6506.818) # With Kopp applying MG's doses for Corn, not

# OT: Only plot areas crossed by Transect
### With Kopp applying MG's doses for Corn, not Beet
# Appl.Mass.g.OT = c(24477.491, 12249.068, 1803.066, 4454.233)
# Appl.Mass.g.OT = c(14648.725, 12249.068, 1803.066, 6307.544) # Friess's, S-15 on transect
# Friess & Kopp applying MG's doses for Corn, not Beet
Appl.Mass.g.OT = c(24477.491, 12249.068, 1803.066, 6307.544)
```

Temperatures and soil moisture after application

The mean and ranges of air temperatures 120 hr. (5 days) after each application were:

- 1st Application: 8.3 (6.7 - 9.2)
- 2nd Application: 9.6 (7.4 - 11.2)
- 3rd Application: 14.4 (10.9 - 17.4)
- 4th Application: 16.9 (14.9 - 19.3)

```
temp_1st = c(6.70, 9.10, 8.40, 8.20, 9.20)
temp_2nd = c(11.00, 11.20, 10.00, 7.40, 8.20)
temp_3rd = c(17.30, 11.10, 10.90, 13.70, 17.40)
temp_4th = c(19.30, 18.70, 17.00, 14.90, 14.90)

temp_list = list(temp_1st, temp_2nd, temp_3rd, temp_4th)

temp_all = Reduce(c,temp_list)

# Mean
mean(temp_all)
```

```
## [1] 12.23
```

```
# Std. Dev:
sd(temp_all)
```

```
## [1] 4.065788
```

Moisture conditions during the same periods where:

```
theta_1st = c(27.40, 30.17, 29.66)
theta_2nd = c(22.43, 23.90, 22.33, 25.90, 30.02, 25.46)
theta_3rd = c(25.30, 29.33, 26.85, 14.37, 17.82, 21.36)
theta_4th = c(14.37, 17.82, 21.36, 27.94, 30.38, 26.87)

theta_list = list(theta_1st, theta_2nd, theta_3rd, theta_4th)

theta_all = Reduce(c,theta_list)

# Mean
mean(theta_all)
```

```
## [1] 24.33524
```

```r
# Std. Dev:
sd(theta_all)
```

```
## [1] 5.025109
```

```r
min(theta_all)
```

```
## [1] 14.37
```

```r
max(theta_all)
```

```
## [1] 30.38
```

```r
# 1st Application (Composite 1):
mean(theta_1st)
```

```
## [1] 29.07667
```

```r
min(theta_1st)
```

```
## [1] 27.4
```

```r
max(theta_1st)
```

```
## [1] 30.17
```

```r
# 2nd Application (Composites 2 & 3):
mean(theta_1st)
```

```
## [1] 29.07667
```

```r
min(theta_1st)
```

```
## [1] 27.4
```

```r
max(theta_1st)
```

```
## [1] 30.17
```

```r
# 3rd Application (Composites 9 & 10):
mean(theta_1st)
```

```
## [1] 29.07667
```

```r
min(theta_1st)
```

```
## [1] 27.4
```

```r
max(theta_1st)
```

```
## [1] 30.17
```

```r
# 4th Application (Composites 10 & 11):
mean(theta_4th)
```

```
## [1] 23.12333
```

```r
min(theta_4th)
```

```
## [1] 14.37
```

```r
max(theta_4th)
```

```
## [1] 30.38
```

Initial soil concentrations (Open Rayleigh requirements)

Open system Rayleigh calculations require estimation of cumulative initial concentration ($C(a)_{Tr_0}$) after any number of plot applications a taking place in a composite sample (i.e. Transect (Tr)) and given by:

$$C(a)_{Tr_0} = \sum_{a=1}^{A} \sum_{i=1}^{I} C(a)_i \cdot \frac{A_i}{A_{Tr}}$$

where $C(a)_i$ is the soil concentation due to application a in plot i, A_i is the plot area and A_{Tr} the total plot area associated to transect (Tr) (i.e. this is proportional to sampling points along transect, and not extrapolated to areas that the transect did not cross). Note that initial concentrations at each transect will be later extrapolated to the catchment to calculate initial catchment concentrations (bulk), which in turn do take into account the full catchment area.

```
# OT: Only plot areas crossed by Transect

### With Kopp applying MG's doses for Corn, not Beet &
# Matthis applying extra DG's doses for Corn, or using slightly higher MG doses
# Appl.Mass.g.OT = c(27076.406, 12249.068, 1803.066, 4454.233)

Appl.Mass.g.N <- c(8429.434, 7810.101, 0, 5346.189)
Appl.Mass.g.N.OT <- c(8429.434, 7810.101, 0, 3293.605) # Friess with DG
# Appl.Mass.g.N.OT <- c(2528.830, 7810.101, 0, 3293.605) # Friess with MG

Appl.Mass.g.T <- c(6903.610, 3073.636, 1803.066, 0)
Appl.Mass.g.T.OT <- c(2727.322, 3006.507, 1803.066, 0) # Friess with DG
# Appl.Mass.g.T.OT <- c(818.196, 3006.507, 1803.066, 0) # Friess with MG

Appl.Mass.g.S <- c(16337.030, 1432.460, 0, 1160.628)
## Options:
# 1
# Appl.Mass.g.S.OT <- c(13320.736, 1432.460, 0, 1160.628)
Appl.Mass.g.S.OT <- c(13320.736, 1432.460, 0, 3016.294) # Friess's S-15 on transect
# Appl.Mass.g.S.OT <- c(11301.698, 1432.460, 0, 3016.294) # Friess's S-15 on transect, Freiss with MG f

# 2
# Matthis applying DG's doses for Corn, but using MG
# Appl.Mass.g.S.OT <- c(15919.651, 1432.460, 0, 1160.628)

# Initial soil concentration (needed for Rayleigh calculations later)

# Effective area [m2] refers to plot area touched by a transect, not sub-catchment area.
Narea_eff <- 101721.702
Tarea_eff <- 39247.330
Sarea_eff <- 109903.101 # With S-15 (Friess Corn) on Transect

MGplotConc.Corn <- 19.592 # Assume for Friess, as he grew both Corn and Beet
MGplotConc.Beet <- 5.878 # ug/g soil for Mercantor Gold
DGplotConc <- 19.607 # Dual Gold
# MGbutDG.Matthis <- 24.490

### Initial concentrations:

# First applciations
```

```
north_first <-
  # MGplotConc.Beet*(43903.301/Narea_eff) # Friess Area fraction, ug/g
  MGplotConc.Corn*(43903.301/Narea_eff) # Friess Area fraction, ug/g

talweg_first <-
  # MGplotConc.Beet*(14204.800/Tarea_eff) # Friess
  MGplotConc.Corn*(14204.800/Tarea_eff) # Friess
  # DGplotConc*(14204.800/Tarea_eff) # Friess

south_first <-
  # MGplotConc.Beet*(15022.6/Sarea_eff)+ # Friess, S-11
  MGplotConc.Corn*(15022.6/Sarea_eff)+ # Friess, S-11
  # DGplotConc*(15022.6/Sarea_eff)+ # Friess, S-11
  # DGplotConc*(15697.6/Sarea_eff)+ # Friess, S-15  # Now or in May??
  # MGplotConc.Beet*(54313.801/Sarea_eff) # Mathis area/area_tot.S
  DGplotConc*(54313.801/Sarea_eff) # Mathis area/area_tot.S
  #MGbutDG.Matthis*(54313.801/Sarea_eff) # Mathis area/area_tot.S

# Second applications
north_second <-
  north_first+
  MGplotConc.Corn*(9452.500/Narea_eff+ # Kopp, N-4
                     13776.500/Narea_eff+ # Kopp, N-7
                     17448.600/Narea_eff) # Kopp, N-8
talweg_second <-
  talweg_first+
  MGplotConc.Corn*(2965.980/Tarea_eff # Kopp, T-4
                   + 5336.080/Tarea_eff # Kopp, T-7
                   + 7356.830/Tarea_eff) # Kopp, T-8
south_second <-
  south_first +
  MGplotConc.Beet*(24869.100/Sarea_eff) # Burger

# Third applications
north_third <- north_second

talweg_third <-
  talweg_second+
  DGplotConc*(9383.640/Tarea_eff) # Schmitt, T-10

south_third <- south_second

# Fourth applications
north_fourth <-
  north_second+
  # MGplotConc.Corn*(17140.801/Narea_eff) # Speich Corn with MG
  DGplotConc*(17140.801/Narea_eff) # Speich Corn with DG

talweg_fourth <- talweg_third
# south_fourth <- south_second # If Speich's S-70 not in transect
south_fourth <- south_second +
  MGplotConc.Corn*(6040.220/Narea_eff) + # Speich Corn with MG (South Transect)
  DGplotConc*(15697.6/Sarea_eff) # Friess, S-15  # Now or in April??
```

```
applics = as.data.frame(ti)
applics$Appl.Mass.g = Appl.Mass.g
applics$Appl.Mass.g.OT = Appl.Mass.g.OT
applics$Appl.Mass.g.N = Appl.Mass.g.N
applics$Appl.Mass.g.T = Appl.Mass.g.T
applics$Appl.Mass.g.S = Appl.Mass.g.S

applics$Appl.Mass.g.N.OT = Appl.Mass.g.N.OT
applics$Appl.Mass.g.T.OT = Appl.Mass.g.T.OT
applics$Appl.Mass.g.S.OT = Appl.Mass.g.S.OT

applics$iniCo.ug.g.N = c(north_first, north_second, north_third, north_fourth)
applics$iniCo.ug.g.T = c(talweg_first, talweg_second, talweg_third, talweg_fourth)
applics$iniCo.ug.g.S = c(south_first, south_second, south_third, south_fourth)

out.CoIs = merge(out.CoIs, applics, by = "ti", all = T)

out.CoIs$Appl.Mass.g <- ifelse(is.na(out.CoIs$Appl.Mass.g), 0.0, out.CoIs$Appl.Mass.g)
out.CoIs$Appl.Mass.g.OT <- ifelse(is.na(out.CoIs$Appl.Mass.g.OT), 0.0, out.CoIs$Appl.Mass.g.OT)

out.CoIs$Appl.Mass.g.N <- ifelse(is.na(out.CoIs$Appl.Mass.g.N), 0.0, out.CoIs$Appl.Mass.g.N)
out.CoIs$Appl.Mass.g.T <- ifelse(is.na(out.CoIs$Appl.Mass.g.T), 0.0, out.CoIs$Appl.Mass.g.T)
out.CoIs$Appl.Mass.g.S <- ifelse(is.na(out.CoIs$Appl.Mass.g.S), 0.0, out.CoIs$Appl.Mass.g.S)

out.CoIs$Appl.Mass.g.N.OT <- ifelse(is.na(out.CoIs$Appl.Mass.g.N.OT), 0.0, out.CoIs$Appl.Mass.g.N.OT)
out.CoIs$Appl.Mass.g.T.OT <- ifelse(is.na(out.CoIs$Appl.Mass.g.T.OT), 0.0, out.CoIs$Appl.Mass.g.T.OT)
out.CoIs$Appl.Mass.g.S.OT <- ifelse(is.na(out.CoIs$Appl.Mass.g.S.OT), 0.0, out.CoIs$Appl.Mass.g.S.OT)

out.CoIs$timeSinceApp <- NA
for (i in 1:length(out.CoIs$Duration.Hrs)){
  if (out.CoIs[i, ]['Appl.Mass.g'] != 0){
    out.CoIs[i,]['timeSinceApp'] = out.CoIs[i, ]['Duration.Hrs']
  } else {
    out.CoIs[i, ]['timeSinceApp'] = out.CoIs[i ,]['Duration.Hrs'] + out.CoIs[i-1,]['timeSinceApp']
  }
}

out.CoIs$timeSinceApp.N <- NA
for (i in 1:length(out.CoIs$Duration.Hrs)){
  if (out.CoIs[i, ]['Appl.Mass.g.N'] != 0){
    out.CoIs[i,]['timeSinceApp.N'] = out.CoIs[i, ]['Duration.Hrs']
  } else {
    out.CoIs[i, ]['timeSinceApp.N'] = out.CoIs[i ,]['Duration.Hrs'] + out.CoIs[i-1,]['timeSinceApp.N']
  }
}

out.CoIs$timeSinceApp.T <- NA
for (i in 1:length(out.CoIs$Duration.Hrs)){
  if (out.CoIs[i, ]['Appl.Mass.g.T'] != 0){
    out.CoIs[i,]['timeSinceApp.T'] = out.CoIs[i, ]['Duration.Hrs']
  } else {
    out.CoIs[i, ]['timeSinceApp.T'] = out.CoIs[i ,]['Duration.Hrs'] + out.CoIs[i-1,]['timeSinceApp.T']
  }
```

```
}

out.CoIs$timeSinceApp.S <- NA
for (i in 1:length(out.CoIs$Duration.Hrs)){
  if (out.CoIs[i, ]['Appl.Mass.g.S'] != 0){
    out.CoIs[i,]['timeSinceApp.S'] = out.CoIs[i, ]['Duration.Hrs']
  } else {
    out.CoIs[i, ]['timeSinceApp.S'] = out.CoIs[i ,]['Duration.Hrs'] + out.CoIs[i-1,]['timeSinceApp.S']
  }
}

# Not in South
out.CoIs$Appl.Mass.g.NoSo <- out.CoIs$Appl.Mass.g
out.CoIs$Appl.Mass.g.NoSo[which(out.CoIs$ti == as.POSIXct('2016-05-23 18:02:00' , tz="EST"))] <- 0
out.CoIs$timeSinceApp.NoSo <- NA
for (i in 1:length(out.CoIs$Duration.Hrs)){
  if (out.CoIs[i, ]['Appl.Mass.g.NoSo'] != 0){
    out.CoIs[i,]['timeSinceApp.NoSo'] = out.CoIs[i, ]['Duration.Hrs']
  } else {
    out.CoIs[i, ]['timeSinceApp.NoSo'] = out.CoIs[i ,]['Duration.Hrs'] + out.CoIs[i-1,]['timeSinceApp.N
  }
}


out.CoIs$timeSinceApp <- round(out.CoIs$timeSinceApp/24, 1) # Convert to days
out.CoIs$timeSinceApp.NoSo <- round(out.CoIs$timeSinceApp.NoSo/24, 1)
out.CoIs$timeSinceApp.N <- round(out.CoIs$timeSinceApp.N/24, 1) # Convert to days
out.CoIs$timeSinceApp.T <- round(out.CoIs$timeSinceApp.T/24, 1) # Convert to days
out.CoIs$timeSinceApp.S <- round(out.CoIs$timeSinceApp.S/24, 1) # Convert to days

# Cumulative (Continous)
out.CoIs$CumAppMass.g = cumsum(out.CoIs$Appl.Mass.g)
out.CoIs$CumAppMass.g.OT = cumsum(out.CoIs$Appl.Mass.g.OT)
out.CoIs$CumAppMass.g.N = cumsum(out.CoIs$Appl.Mass.g.N)
out.CoIs$CumAppMass.g.T = cumsum(out.CoIs$Appl.Mass.g.T)
out.CoIs$CumAppMass.g.S = cumsum(out.CoIs$Appl.Mass.g.S)
out.CoIs$CumAppMass.g.N.OT = cumsum(out.CoIs$Appl.Mass.g.N.OT)
out.CoIs$CumAppMass.g.T.OT = cumsum(out.CoIs$Appl.Mass.g.T.OT)
out.CoIs$CumAppMass.g.S.OT = cumsum(out.CoIs$Appl.Mass.g.S.OT)

out.CoIs$iniCo.ug.g.N = na.locf(out.CoIs$iniCo.ug.g.N)
out.CoIs$iniCo.ug.g.T = na.locf(out.CoIs$iniCo.ug.g.T)
out.CoIs$iniCo.ug.g.S = na.locf(out.CoIs$iniCo.ug.g.S)
```

Balance

```
# Balance
out.CoIs$BalMassDisch.g = out.CoIs$CumAppMass.g - out.CoIs$CumOutMELsm.g

# Mass fraction
massOUT = tail(out.CoIs$CumOutSmeto.g, n=1)
MELsmOUT = tail(out.CoIs$CumOutMELsm.g, n=1)
```

```
TotAppl = tail(out.CoIs$CumAppMass.g, n=1)

out.CoIs$prctMassOut = (out.CoIs$TotSMout.g / massOUT)
out.CoIs$FracDeltaOut = (out.CoIs$TotSMout.g / massOUT)*out.CoIs$diss.d13C
out.CoIs$FracDeltaOut = ifelse(is.na(out.CoIs$FracDeltaOut), 0.0, out.CoIs$FracDeltaOut)

BulkDeltaOut = sum(out.CoIs$FracDeltaOut)
```

The total mass discharged (up to Week 15) and bulk isotope signature (up to week 11) was:

```
# Cummulative S-metolachlor [g] discharged (before correction)
cat("SM mass sampled: " , as.character(91.10687))
```

```
## SM mass sampled:  91.10687
```

```
# Cummulative S-metolachlor [g] discharged
cat("SM mass sampled and non-sampled: ",  as.character(massOUT))
```

```
## SM mass sampled and non-sampled:  140.39430171711
```

```
# Cummulative MEL-sm [g] discharged
cat("MEL-sm [g] sampled and non-sampled: ",  as.character(MELsmOUT))
```

```
## MEL-sm [g] sampled and non-sampled:  4311.9545467332
```

```
cat("% Mass applied in discahrge [MEL-sm]: ",  (MELsmOUT/TotAppl)*100)
```

```
## % Mass applied in discahrge [MEL-sm]:  8.245261
```

```
# Bulk isotope signature
BulkDeltaOut
```

```
## [1] -19.06464
```

Save files

```
names(out.CoIs)[names(out.CoIs) == "Event"] <- "Peak"

out.CoIs$Events <- as.factor(c("0-1", "0-2", "0-3",
                           "1-1", "1-2", "1-3",
                           "2-1", "2-2", "2-3",
                           "3-1",
                           "4-1", "4-2", "4-3", "4-4", "4-5",
                           "5-1",
                           "6-1", "6-2", "6-3",
                           "7-1",
                           "8-1", "8-2", "8-3",
                           "9-1", "9-2", "9-3", "9-4", "9-5",
                           "10-1", "10-2", "10-3", "10-4", "10-5",
                           "11-1",
                           "12-1", "12-2", "12-3",
                           "13-1",
                           "14-1",
                           "15-1", "15-2", "15-3", "15-4",
                           "16-1", "16-2",
                           "17-1", "17-2",
```

```
                        "18-1", "18-2", "18-3", "18-4"))

# Adding a Weeks column for labelling
out.CoIs$WeekSubWeek <- as.character(out.CoIs$WeekSubWeek)
Split <- strsplit(out.CoIs$WeekSubWeek, "-", fixed = TRUE)
out.CoIs$Weeks <- sapply(Split, "[", 1)

Split2 <- strsplit(as.character(out.CoIs$Events), "-", fixed = T)
out.CoIs$Event <- as.factor(sapply(Split2, "[", 1))

out.CoIs$WeekSubWeek <- factor(out.CoIs$WeekSubWeek, levels = unique(out.CoIs$WeekSubWeek))
out.CoIs$Weeks <- factor(out.CoIs$Weeks, levels = unique(out.CoIs$Weeks))

out.CoIs$Events <- factor(out.CoIs$Events, levels = unique(out.CoIs$Events))
out.CoIs$Event <- factor(out.CoIs$Event, levels = unique(out.CoIs$Event))

head(out.CoIs)
```

```
##                    ti WeekSubWeek                  tf     iflux     fflux
## 1 2016-03-25 00:04:00       W0-0x 2016-03-25 12:02:00  1.248600  1.129227
## 2 2016-03-25 12:04:00        W0-1 2016-03-28 22:36:00  1.124382  1.313125
## 3 2016-03-28 22:38:00       W0-2x 2016-03-30 12:16:00  1.308100  1.456349
## 4 2016-03-30 12:18:00        W1-1 2016-03-31 15:34:00  1.456080 16.445436
## 5 2016-03-31 15:36:00        W1-2 2016-04-01 14:44:00 16.334349 15.184536
## 6 2016-04-01 14:46:00       W1-3x 2016-04-05 15:06:00 15.203629  5.856380
##   changeflux      maxQ      minQ  dryHrsIni dryHrsMax dryHrsAve
## 1 -0.1193728  1.248600  1.118296 0.01666667  2.750000 0.7449537
## 2  0.1887431  1.380388  1.082199 0.03333333 24.516667 7.8272574
## 3  0.1482496  1.637782  0.929055 0.26666667 13.316667 4.8591888
## 4 14.9893566 38.399790  1.448977 0.11666667  4.200000 1.2885633
## 5 -1.1498131 18.668972 13.201113 4.21666667  5.433333 1.3142446
## 6 -9.3472489 15.895640  5.471042 3.41666667 29.716667 9.4699181
##   noEventHrsIni noEventHrsMax noEventHrsAve Duration.Hrs  chExtreme Peak
## 1    0.01666667      6.000000      3.008333     11.96667 -0.1303036   NA
## 2    6.01666667     47.283333     26.650000     82.53333  0.2560062   NA
## 3   47.30000000     66.116667     56.708333     37.63333  0.3296817   NA
## 4   66.13333333     72.100000     30.395503     27.26667 36.9437102    1
## 5    1.65000000      6.366667      3.329089     23.13333 -3.1332355   NA
## 6    6.26666667     54.433333     30.350000     96.33333 -9.7325862   NA
##    Markers TimeDiff AveDischarge.m3.h Volume.m3 Sampled.Hrs     Sampled
## 1       NA     <NA>          1.204775  14.41714    11.96667 Not Sampled
## 2       NA     <NA>          1.213511 100.15508    82.53333     Sampled
## 3       NA     <NA>          1.284719  48.34827    37.63333 Not Sampled
## 4 16.88972       24         14.316647 390.36726    27.26667     Sampled
## 5       NA     <NA>         15.529299 359.24445    23.13333     Sampled
## 6       NA     <NA>          9.107720 877.37700    96.33333 Not Sampled
##   CumRain.mm RainInt.mmhr Conc.mug.L  Conc.SD Vol.SPE.L Conc.in500uL
## 1        2.8   0.23398329  0.2456594 0.019310      0.57           NA
## 2        7.6   0.09208401  0.2456594 0.019310      0.57     140.0258
## 3        7.6   0.20194863  3.5169528 0.154365        NA           NA
## 4       16.8   0.61613692  6.7882463 0.289420      1.91   12965.5505
## 5        6.0   0.25936599  6.5609982 0.190640      1.91   12531.5066
## 6        9.4   0.09757785  8.0026500 0.262090        NA           NA
##   OXA_mean OXA_SD ESA_mean ESA_SD N.x diss.d13C   SD.d13C N_d13C.diss
```

```
## 1     74.0     39     45.0   59.0  NA        NA        NA          NA
## 2     74.0     39     45.0   59.0  NA        NA        NA          NA
## 3     71.5     42     58.5   58.0  NA        NA        NA          NA
## 4     69.0     45     72.0   57.0   3 -31.46667 0.1154701           3
## 5     70.0     22     70.0   25.0   3 -31.66667 0.1527525           3
## 6     59.0     31     76.5   38.5  NA        NA        NA          NA
##   MES.mg.L MES.sd MO.mg.L Conc.Solids.mug.gMES Conc.Solids.ug.gMES.SD N.y
## 1       NA     NA      NA            0.6447290             0.02323755  NA
## 2 53.44444     NA   0e+00            0.6447290             0.02323755  NA
## 3       NA     NA      NA            0.3853094             0.02515062  NA
## 4 62.50000     NA   1e-03            0.1258897             0.02706369  NA
## 5 22.50000     NA   1e-04            0.4357872             0.12323706  NA
## 6       NA     NA      NA            0.2575699             0.06396039  NA
##   filt.d13C filt.SD.d13C DD13C.diss DD13C.filt ExpMES.Kg DissSmeto.mg
## 1        NA           NA         NA         NA  5.352733     3.541705
## 2        NA           NA         NA         NA  5.352733    24.604033
## 3        NA           NA         NA         NA 14.875343   170.038598
## 4        NA           NA  0.8333333         NA 24.397953  2649.909084
## 5        NA           NA  0.6333333         NA  8.083000  2357.002211
## 6        NA           NA         NA         NA  7.935755  7021.341115
##   DissSmeto.mg.SD DissSmeto.g DissSmeto.g.SD DissOXA.mg DissOXA.mg.SD
## 1       0.2783949 0.003541705   0.0002783949   1066.868      562.2683
## 2       1.9339946 0.024604033   0.0019339946   7411.476     3906.0481
## 3       7.4632812 0.170038598   0.0074632812   3456.902     2030.6275
## 4     112.9800910 2.649909084   0.1129800910  26935.341    17566.5265
## 5      68.4863626 2.357002211   0.0684863626  25147.112     7903.3780
## 6     229.9517390 7.021341115   0.2299517390  51765.243    27198.6871
##   DissOXA.g DissOXA.g.SD DissESA.mg DissESA.mg.SD  DissESA.g DissESA.g.SD
## 1  1.066868    0.5622683   648.7711       850.611  0.6487711     0.850611
## 2  7.411476    3.9060481  4506.9786      5909.150  4.5069786     5.909150
## 3  3.456902    2.0306275  2828.3740      2804.200  2.8283740     2.804200
## 4 26.935341   17.5665265 28106.4424     22250.934 28.1064424    22.250934
## 5 25.147112    7.9033780 25147.1117      8981.111 25.1471117     8.981111
## 6 51.765243   27.1986871 67119.3408     33779.015 67.1193408    33.779015
##   FiltSmeto.mg FiltSmeto.mg.SD FiltSmeto.g FiltSmeto.g.SD TotSMout.mg
## 1     3.451062       0.1243844 0.003451062   0.0001243844    6.992766
## 2     3.451062       0.1243844 0.003451062   0.0001243844   28.055095
## 3     5.731609       0.3741240 0.005731609   0.0003741240  175.770206
## 4     3.071452       0.6602985 0.003071452   0.0006602985 2652.980536
## 5     3.522468       0.9961252 0.003522468   0.0009961252 2360.524679
## 6     2.044012       0.5075740 0.002044012   0.0005075740 7023.385126
##   TotSMout.mg.SD  TotSMout.g TotSMout.g.SD  FracDiss     FracFilt
## 1      0.2156098 0.006992766  0.0002156098 0.5064812 0.4935188249
## 2      1.3703661 0.028055095  0.0013703661 0.8769898 0.1230101642
## 3      5.2839633 0.175770206  0.0052839633 0.9673915 0.0326085349
## 4     79.8903528 2.652980536  0.0798903528 0.9988423 0.0011577363
## 5     48.4322936 2.360524679  0.0484322936 0.9985078 0.0014922393
## 6    162.6008301 7.023385126  0.1626008301 0.9997090 0.0002910294
##      MELsm.g MELsm.g.SD CumOutDiss.g CumOutFilt.g CumOutSmeto.g
## 1   1.650379  0.5367746  0.003541705  0.003451062   0.006992766
## 2  11.444574  3.7289448  0.028145738  0.006902124   0.035047862
## 3   6.126961  1.8352060  0.198184336  0.012633733   0.210818068
## 4  54.256272 15.1295476  2.848093419  0.015705185   2.863798604
## 5  49.595048  6.4410275  5.205095630  0.019227652   5.224323282
```

```
## 6 117.495938 23.1814377 12.226436745  0.021271664  12.247708409
##   CumOutMELsm.g Appl.Mass.g Appl.Mass.g.OT Appl.Mass.g.N Appl.Mass.g.T
## 1      1.650379    31670.07       24477.49      8429.434       6903.61
## 2     13.094954        0.00           0.00         0.000          0.00
## 3     19.221914        0.00           0.00         0.000          0.00
## 4     73.478186        0.00           0.00         0.000          0.00
## 5    123.073234        0.00           0.00         0.000          0.00
## 6    240.569172        0.00           0.00         0.000          0.00
##   Appl.Mass.g.S Appl.Mass.g.N.OT Appl.Mass.g.T.OT Appl.Mass.g.S.OT
## 1      16337.03         8429.434         2727.322         13320.74
## 2          0.00            0.000            0.000             0.00
## 3          0.00            0.000            0.000             0.00
## 4          0.00            0.000            0.000             0.00
## 5          0.00            0.000            0.000             0.00
## 6          0.00            0.000            0.000             0.00
##   iniCo.ug.g.N iniCo.ug.g.T iniCo.ug.g.S timeSinceApp timeSinceApp.N
## 1     8.455948     7.090939     12.36774          0.5            0.5
## 2     8.455948     7.090939     12.36774          3.9            3.9
## 3     8.455948     7.090939     12.36774          5.5            5.5
## 4     8.455948     7.090939     12.36774          6.6            6.6
## 5     8.455948     7.090939     12.36774          7.6            7.6
## 6     8.455948     7.090939     12.36774         11.6           11.6
##   timeSinceApp.T timeSinceApp.S Appl.Mass.g.NoSo timeSinceApp.NoSo
## 1            0.5            0.5         31670.07               0.5
## 2            3.9            3.9             0.00               3.9
## 3            5.5            5.5             0.00               5.5
## 4            6.6            6.6             0.00               6.6
## 5            7.6            7.6             0.00               7.6
## 6           11.6           11.6             0.00              11.6
##   CumAppMass.g CumAppMass.g.OT CumAppMass.g.N CumAppMass.g.T
## 1     31670.07        24477.49       8429.434        6903.61
## 2     31670.07        24477.49       8429.434        6903.61
## 3     31670.07        24477.49       8429.434        6903.61
## 4     31670.07        24477.49       8429.434        6903.61
## 5     31670.07        24477.49       8429.434        6903.61
## 6     31670.07        24477.49       8429.434        6903.61
##   CumAppMass.g.S CumAppMass.g.N.OT CumAppMass.g.T.OT CumAppMass.g.S.OT
## 1       16337.03          8429.434          2727.322          13320.74
## 2       16337.03          8429.434          2727.322          13320.74
## 3       16337.03          8429.434          2727.322          13320.74
## 4       16337.03          8429.434          2727.322          13320.74
## 5       16337.03          8429.434          2727.322          13320.74
## 6       16337.03          8429.434          2727.322          13320.74
##   BalMassDisch.g  prctMassOut FracDeltaOut Events Weeks Event
## 1       31668.42 4.980805e-05    0.0000000    0-1    W0     0
## 2       31656.98 1.998307e-04    0.0000000    0-2    W0     0
## 3       31650.85 1.251975e-03    0.0000000    0-3    W0     0
## 4       31596.59 1.889664e-02   -0.5946143    1-1    W1     1
## 5       31547.00 1.681354e-02   -0.5324286    1-2    W1     1
## 6       31429.50 5.002614e-02    0.0000000    1-3    W1     1
```

```
write.csv2(out.CoIs,
           'Data/WeeklyHydroContam_R.csv', row.names = F)
sum(is.na(out.CoIs$maxQ))
```

```
## [1] 0
```

```
# out.CoIs = read.csv2("Data/WeeklyHydroContam_R.csv")
# out.CoIs$ti = as.POSIXct(out.CoIs$ti, "%Y-%m-%d %H:%M", tz = "EST")
```