# Mass Discharge - Outlet Alteck. 2016

*PAZ*

*27 octobre 2016*

## 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")
```

```
## Warning: package 'plotly' was built under R version 3.3.3
```

## 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] "D:/Documents/these_pablo/Alteckendorf2016/HydrologicalMonitoring"
```

## Lab and reference values

```
# Pure and cuve isotope average
d13Co = -32.25

# Lab enrichment:
# epsilon = -1.61

# Lab enrichment:
# Alteck
#epsilon_max = -1.5 # +/- 0.3 (@ 20C, 20% vwc)
#epsilon_min = -2.0 # +/- 0.2 (@ 20C, 40% vwc)
#epsilon_mean = -1.75

# Ehssan values:
epsilon_max = -1.8
epsilon_min = -2.6
epsilon_mean = -2.2 # Â± 0.4

# Field values, after dilution correction (Van Breukelen 2008):
# Calculated in Book 9.1
epsilonField_max = -1.7 + 0.33
epsilonField_min = -1.7 - 0.33
epsilonField_mean = -1.7 # Â± 0.33
```

## 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", header = T)
outletConc$ID4 <- as.character(outletConc$ID4)
outletConc <- outletConc[outletConc$ID4 != "J+7", ]
outletConc <- outletConc[,c("WeekSubWeek", "Conc.mug.L", "Conc.SD")]
head(outletConc)
```

```
##   WeekSubWeek Conc.mug.L Conc.SD
## 1        W0-1  0.2456594 0.01931
## 2        W1-1  6.7882463 0.28942
## 3        W1-2  6.5609982 0.19064
## 4        W2-1  9.4443019 0.33354
## 5        W2-2  1.0421883 0.03904
## 6        W3-1  8.8357358 0.47086
```

```
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

head(sd_temp)
```

```
##      MOXA.ugL  MESA.ugL ESAOXA_SD ESAOXA_Mean
## 2   1.1414453 3.4972206        SD     AO-W0-1
## 4  10.1852510 3.0369845        SD     AO-W1-1
## 6   0.2430544 0.8533820        SD     AO-W1-2
## 8   1.1526489 2.8261924        SD     AO-W2-1
## 10  0.6100011 0.1910419        SD     AO-W2-2
## 12  2.6589421 0.3268637        SD     AO-W3-1
```

```
head(means_temp)
```

```
##      MOXA.ugL MESA.ugL ESAOXA_SD ESAOXA_Mean
## 1    4.824094 18.05531      <NA>     AO-W0-1
## 3   30.531235 45.98364      <NA>     AO-W1-1
## 5   32.492465 41.28052      <NA>     AO-W1-2
## 7  104.541255 98.56782      <NA>     AO-W2-1
## 9   26.885849 51.95245      <NA>     AO-W2-2
## 11  45.080673 24.04717      <NA>     AO-W3-1
```

```
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  4.824094  1.14144531 18.05531 3.4972206
## 2        W1-1 30.531235 10.18525095 45.98364 3.0369845
```

```
## 3        W1-2 32.492465  0.24305444 41.28052 0.8533820
## 4       W10-1 21.311423  0.05168437 82.87549 1.8167218
## 5       W10-2 13.095046  0.17703516 12.02387 0.3057521
## 6       W10-3 45.605808  1.92663562 11.31492 0.1763479
```

### Isotope data

```
# 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-W11-1-1_.dxf",..: 13 14 15 16 17 18 52 53 54 64 ..
##  $ 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"
```

```
outletIso$DD13 <- outletIso$d.13C.12C - -32.253

# 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)


# Hydrochemistrty
out.CoIs = merge(out.CoIs, hydroChem, 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] 7
```

```
# 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("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)), ]

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 $\Delta t$ 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
```

## 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)
```

## Application dates and masses

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)
```

## 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:  140.392784355072
```

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

```
## MEL-sm [g] sampled and non-sampled:  3096.82107110135
```

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

```
## % Mass applied in discahrge [MEL-sm]:  5.921699
```

```
# Bulk isotope signature
BulkDeltaOut
```

```
## [1] -19.06529
```

## 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  OXA_mean     OXA_SD
## 1        2.8   0.23398329  0.2456594 0.019310  4.824094  1.1414453
## 2        7.6   0.09208401  0.2456594 0.019310  4.824094  1.1414453
## 3        7.6   0.20194863  3.5169528 0.154365 17.677665  5.6633481
## 4       16.8   0.61613692  6.7882463 0.289420 30.531235 10.1852510
## 5        6.0   0.25936599  6.5609982 0.190640 32.492465  0.2430544
## 6        9.4   0.09757785  8.0026500 0.262090 68.516860  0.6978517
##   ESA_mean   ESA_SD N.x diss.d13C   SD.d13C N_d13C.diss MES.mg.L MES.sd
## 1 18.05531 3.497221  NA        NA        NA          NA       NA     NA
## 2 18.05531 3.497221  NA        NA        NA          NA 53.44444     NA
## 3 32.01948 3.267103  NA        NA        NA          NA       NA     NA
## 4 45.98364 3.036985   3 -31.51000 0.1039230           3 62.50000     NA
## 5 41.28052 0.853382   3 -31.66333 0.1517674           3 22.50000     NA
## 6 69.92417 1.839787  NA        NA        NA          NA       NA     NA
##   MO.mg.L Conc.Solids.mug.gMES Conc.Solids.ug.gMES.SD N.y filt.d13C
## 1      NA            0.6447290             0.02323755  NA        NA
## 2   0e+00            0.6447290             0.02323755  NA        NA
## 3      NA            0.3853094             0.02515062  NA        NA
## 4   1e-03            0.1258897             0.02706369  NA        NA
## 5   1e-04            0.4357872             0.12323706  NA        NA
## 6      NA            0.2575699             0.06396039  NA        NA
##   filt.SD.d13C DD13C.diss DD13C.filt NH4.mM TIC.ppm.filt   Cl.mM NO3...mM
## 1           NA         NA         NA     NA           NA      NA       NA
## 2           NA         NA         NA     NA           NA      NA       NA
## 3           NA         NA         NA     NA           NA      NA       NA
## 4           NA  0.7400000         NA   0.05         51.8    1.48      616
## 5           NA  0.5866667         NA     NA         44.8 1574.00      778
## 6           NA         NA         NA     NA           NA      NA       NA
##   PO4..mM NPOC.ppm TIC.ppm.unfilt TOC.ppm.unfilt 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      4.0           44.8            4.7 24.397953  2649.909084
## 5      NA      4.4           26.4            5.4  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    69.54963      16.45637
## 2       1.9339946 0.024604033   0.0019339946   483.15756     114.32155
## 3       7.4632812 0.170038598   0.0074632812   854.68456     273.81310
## 4     112.9800910 2.649909084   0.1129800910 11918.39439    3975.98846
## 5      68.4863626 2.357002211   0.0684863626 11672.73795      87.31596
## 6     229.9517390 7.021341115   0.2299517390 60115.11746     612.27900
##     DissOXA.g DissOXA.g.SD DissESA.mg DissESA.mg.SD  DissESA.g
## 1  0.06954963   0.01645637   260.3058      50.41991  0.2603058
## 2  0.48315756   0.11432155  1808.3308     350.26441  1.8083308
## 3  0.85468456   0.27381310  1548.0863     157.95877  1.5480863
## 4 11.91839439   3.97598846 17950.5083    1185.53932 17.9505083
## 5 11.67273795   0.08731596 14829.7964     306.57276 14.8297964
## 6 60.11511746   0.61227900 61349.8588    1614.18699 61.3498588
##   DissESA.g.SD FiltSmeto.mg FiltSmeto.mg.SD FiltSmeto.g FiltSmeto.g.SD
## 1   0.05041991     3.451062       0.1243844 0.003451062   0.0001243844
## 2   0.35026441     3.451062       0.1243844 0.003451062   0.0001243844
## 3   0.15795877     5.731609       0.3741240 0.005731609   0.0003741240
```

```
## 4   1.18553932     3.071452       0.6602985 0.003071452   0.0006602985
## 5   0.30657276     3.522468       0.9961252 0.003522468   0.0009961252
## 6   1.61418699     2.044012       0.5075740 0.002044012   0.0005075740
##   TotSMout.mg TotSMout.mg.SD  TotSMout.g TotSMout.g.SD  FracDiss
## 1    6.992766      0.2156098 0.006992766  0.0002156098 0.5064812
## 2   28.055095      1.3703661 0.028055095  0.0013703661 0.8769898
## 3  175.770206      5.2839633 0.175770206  0.0052839633 0.9673915
## 4 2652.980536     79.8903528 2.652980536  0.0798903528 0.9988423
## 5 2360.524679     48.4322936 2.360524679  0.0484322936 0.9985078
## 6 7023.385126    162.6008301 7.023385126  0.1626008301 0.9997090
##       FracFilt     MELsm.g MELsm.g.SD CumOutDiss.g CumOutFilt.g
## 1 0.4935188249   0.3021264 0.02689497  0.003541705  0.003451062
## 2 0.1230101642   2.0783329 0.18683762  0.028145738  0.006902124
## 3 0.0326085349   2.3790960 0.17885971  0.198184336  0.012633733
## 4 0.0011577363  30.2413655 2.40621294  2.848093419  0.015705185
## 5 0.0014922393  27.0082117 0.16340841  5.205095630  0.019227652
## 6 0.0002910294 121.0040582 0.88525127 12.226436745  0.021271664
##   CumOutSmeto.g CumOutMELsm.g Appl.Mass.g Appl.Mass.g.OT Appl.Mass.g.N
## 1   0.006992766     0.3021264    31670.07       24477.49      8429.434
## 2   0.035047862     2.3804594        0.00           0.00         0.000
## 3   0.210818068     4.7595554        0.00           0.00         0.000
## 4   2.863798604    35.0009209        0.00           0.00         0.000
## 5   5.224323282    62.0091326        0.00           0.00         0.000
## 6  12.247708409   183.0131909        0.00           0.00         0.000
##   Appl.Mass.g.T Appl.Mass.g.S Appl.Mass.g.N.OT Appl.Mass.g.T.OT
## 1       6903.61      16337.03         8429.434         2727.322
## 2          0.00          0.00            0.000            0.000
## 3          0.00          0.00            0.000            0.000
## 4          0.00          0.00            0.000            0.000
## 5          0.00          0.00            0.000            0.000
## 6          0.00          0.00            0.000            0.000
##   Appl.Mass.g.S.OT iniCo.ug.g.N iniCo.ug.g.T iniCo.ug.g.S timeSinceApp
## 1         13320.74     8.455948     7.090939     12.36774          0.5
## 2             0.00     8.455948     7.090939     12.36774          3.9
## 3             0.00     8.455948     7.090939     12.36774          5.5
## 4             0.00     8.455948     7.090939     12.36774          6.6
## 5             0.00     8.455948     7.090939     12.36774          7.6
## 6             0.00     8.455948     7.090939     12.36774         11.6
##   timeSinceApp.N timeSinceApp.T timeSinceApp.S Appl.Mass.g.NoSo
## 1            0.5            0.5            0.5         31670.07
## 2            3.9            3.9            3.9             0.00
## 3            5.5            5.5            5.5             0.00
## 4            6.6            6.6            6.6             0.00
## 5            7.6            7.6            7.6             0.00
## 6           11.6           11.6           11.6             0.00
##   timeSinceApp.NoSo CumAppMass.g CumAppMass.g.OT CumAppMass.g.N
## 1               0.5     31670.07        24477.49       8429.434
## 2               3.9     31670.07        24477.49       8429.434
## 3               5.5     31670.07        24477.49       8429.434
## 4               6.6     31670.07        24477.49       8429.434
## 5               7.6     31670.07        24477.49       8429.434
## 6              11.6     31670.07        24477.49       8429.434
##   CumAppMass.g.T CumAppMass.g.S CumAppMass.g.N.OT CumAppMass.g.T.OT
## 1        6903.61       16337.03          8429.434          2727.322
```

```
## 2        6903.61       16337.03          8429.434          2727.322
## 3        6903.61       16337.03          8429.434          2727.322
## 4        6903.61       16337.03          8429.434          2727.322
## 5        6903.61       16337.03          8429.434          2727.322
## 6        6903.61       16337.03          8429.434          2727.322
##   CumAppMass.g.S.OT BalMassDisch.g  prctMassOut FracDeltaOut Events Weeks
## 1          13320.74       31669.77 4.980859e-05    0.0000000    0-1    W0
## 2          13320.74       31667.69 1.998329e-04    0.0000000    0-2    W0
## 3          13320.74       31665.31 1.251989e-03    0.0000000    0-3    W0
## 4          13320.74       31635.07 1.889684e-02   -0.5954396    1-1    W1
## 5          13320.74       31608.06 1.681372e-02   -0.5323784    1-2    W1
## 6          13320.74       31487.06 5.002668e-02    0.0000000    1-3    W1
##   Event
## 1     0
## 2     0
## 3     0
## 4     1
## 5     1
## 6     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")
```