Mass Discharge - Outlet Alteck. 2016

PAZ

27 octobre 2016

Purpose

This file computes the discharged mass observed at the outlet. To do that it imports lab results for isotopes (^{13}C) and s-metolachlor concentrations, as well as the weekly discharge summary.

Imports:

- **WeeklyHydro_R.csv** (R generated)
- **fluxAlteck2016_R.csv** (R generated)
- **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

```
# 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 # ± 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 # ± 0.33
```

Outlet Data - Alteckendorf 2016

1. 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
```

```
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      dryHrs Duration.Hrs  chExtreme Event
## 1 -0.1193728  1.248600  1.118296  0.01666667     11.96667 -0.1303036    NA
## 2  0.1887431  1.380388  1.082199  6.01666667     82.53333  0.2560062    NA
## 3  0.1482496  1.637782  0.929055 47.30000000     37.63333  0.3296817    NA
## 4 14.9893566 38.399790  1.448977 66.13333333     27.26667 36.9437102     1
```

```
## 5 -1.1498131 18.668972 13.201113  1.65000000     23.13333 -3.1332355    NA
## 6 -9.3472489 15.895640  5.471042  6.26666667     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>
```

2. 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
```

3. Isotope data

Isotopes selected where cleaned according to the following rules:

a) The isotope shift was not largely beyond (2x) Streitwieser theoretical limits (i.e. > 10)
b) Isotope shift was non-negative
c) Nanograms of carbon > 2.0.

```
# 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"
```

```
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" ...
```

4. 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

1. 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), ]
```

2. 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
```

Fork! Prepare Data for C-Q Hysteresis curves

```
CQdata <- out.CoIs[with(out.CoIs, order(ti)), ]
CQdata$FlowType <- ifelse(is.na(CQdata$Event), "Fall", "Peak")
CQdata$Event[1:3]<- 0
CQdata$EventMark <- NA

CQdata$EventMark <- na.locf(CQdata$Event)
```

```r
CQdata$EventMark <- ifelse(is.na(CQdata$Event), CQdata$EventMark, CQdata$EventMark*10)
CQdata$Row <- seq.int(nrow(CQdata))

cq1 <- subset(CQdata[1:6, ])

cq1 <- cq1[cq1$Sampled != 'Not Sampled', ]

str(cq1)
```

```
## 'data.frame':    3 obs. of  50 variables:
##  $ WeekSubWeek           : Factor w/ 58 levels "W0-0x","W0-1",..: 2 4 5
##  $ ti                    : POSIXct, format: "2016-03-25 12:04:00" "2016-03-30 12:18:00" ...
##  $ tf                    : POSIXct, format: "2016-03-28 22:36:00" "2016-03-31 15:34:00" ...
##  $ iflux                 : num  1.12 1.46 16.33
##  $ fflux                 : num  1.31 16.45 15.18
##  $ changeflux            : num  0.189 14.989 -1.15
##  $ maxQ                  : num  1.38 38.4 18.67
##  $ minQ                  : num  1.08 1.45 13.2
##  $ dryHrs                : num  6.02 66.13 1.65
##  $ Duration.Hrs          : num  82.5 27.3 23.1
##  $ chExtreme             : num  0.256 36.944 -3.133
##  $ Event                 : num  0 1 NA
##  $ Markers               : num  NA 16.9 NA
##  $ TimeDiff              : Factor w/ 18 levels "106","136","150",..: NA 10 NA
##  $ AveDischarge.m3.h     : num  1.21 14.32 15.53
##  $ Volume.m3             : num  100 390 359
##  $ Sampled.Hrs           : num  82.5 27.3 23.1
##  $ Sampled               : Factor w/ 2 levels "Not Sampled",..: 2 2 2
##  $ Conc.mug.L            : num  0.246 6.788 6.561
##  $ Conc.SD               : num  0.0193 0.2894 0.1906
##  $ OXA_mean              : num  4.82 30.53 32.49
##  $ OXA_SD                : num  1.141 10.185 0.243
##  $ ESA_mean              : num  18.1 46 41.3
##  $ ESA_SD                : num  3.497 3.037 0.853
##  $ N.x                   : int  NA 3 3
##  $ diss.d13C             : num  NA -31.5 -31.7
##  $ SD.d13C               : num  NA 0.104 0.152
##  $ N_d13C.diss           : int  NA 3 3
##  $ MES.mg.L              : num  53.4 62.5 22.5
##  $ MES.sd                : num  NA NA NA
##  $ MO.mg.L               : num  0e+00 1e-03 1e-04
##  $ Conc.Solids.mug.gMES  : num  0.645 0.126 0.436
##  $ Conc.Solids.ug.gMES.SD: num  0.0232 0.0271 0.1232
##  $ N.y                   : int  NA NA NA
##  $ filt.d13C             : num  NA NA NA
##  $ filt.SD.d13C          : num  NA NA NA
##  $ DD13C.diss            : num  NA 0.74 0.587
##  $ DD13C.filt            : num  NA NA NA
##  $ NH4.mM                : num  NA 0.05 NA
##  $ TIC.ppm.filt          : num  NA 51.8 44.8
##  $ Cl.mM                 : num  NA 1.48 1574
##  $ NO3...mM              : num  NA 616 778
##  $ PO4..mM               : int  NA NA NA
##  $ NPOC.ppm              : num  NA 4 4.4
```

```
##  $ TIC.ppm.unfilt        : num  NA 44.8 26.4
##  $ TOC.ppm.unfilt        : num  NA 4.7 5.4
##  $ ExpMES.Kg             : num  5.35 24.4 8.08
##  $ FlowType              : chr  "Fall" "Peak" "Fall"
##  $ EventMark             : num  0 10 1
##  $ Row                   : int  2 4 5
```

```
#p <- ggplot(cq1) +
#  geom_point(aes(x=AveDischarge.m3.h, y=Conc.mug.L), colour="black") +
#  geom_polygon(aes(x=AveDischarge.m3.h, y=Conc.mug.L), colour="black", fill = NA) +

#  geom_text(data = cq1,
#            aes(x=AveDischarge.m3.h, y=Conc.mug.L, label=FlowType), hjust=1.5, vjust=0.5, size = 2)
# p

#p <- ggplotly(p)
#p
```

Section to UPDATE!!!

3. Weekly exported S-metolachlor mass (mg)

This section converts the observed S-metolachlor concentrations to [mg] in dissolved water and suspended solids. For non-sampled 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!!

```
# Assume first observation is equivalent to second for all measured values
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)
```

4. 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)

To compute initial concentration needed for Rayleigh calculations, the application rates are used to derive the respective concentration at each plot C_i, plot area A and the effective transect area $A_t r$ (i.e. proportional to sampling points along transect, not extrapolated area represented by transect within entire catchment).

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.

$$\sum_i C_i \cdot \frac{A_i}{A_{tr}}$$

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


### 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
Appl.Mass.g.OT = c(24477.491, 12249.068, 1803.066, 6307.544) # Friess & Kopp applying MG's doses for Co

### 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.
# Need this to calculate initial concentration.
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)
```

Section to UPDATE!!!

5. This section is based on approximate carried-last-observation for the observed concentration data (if no model has been conducted yet).

Also, mass equivalent loads are calculated such that:

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

```
# First simulate a mass out to deal with missing values
# Option 1, just assume 0.0

# 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

# 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)

# 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
```

6. Testing a regression tree (ommitted for now)

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)
```

```r
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      dryHrs Duration.Hrs  chExtreme Peak
## 1 -0.1193728  1.248600  1.118296  0.01666667     11.96667 -0.1303036   NA
## 2  0.1887431  1.380388  1.082199  6.01666667     82.53333  0.2560062   NA
## 3  0.1482496  1.637782  0.929055 47.30000000     37.63333  0.3296817   NA
## 4 14.9893566 38.399790  1.448977 66.13333333     27.26667 36.9437102    1
## 5 -1.1498131 18.668972 13.201113  1.65000000     23.13333 -3.1332355   NA
## 6 -9.3472489 15.895640  5.471042  6.26666667     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
##   Conc.mug.L  Conc.SD  OXA_mean     OXA_SD ESA_mean   ESA_SD N.x diss.d13C
## 1  0.2456594 0.019310  4.824094  1.1414453 18.05531 3.497221  NA        NA
## 2  0.2456594 0.019310  4.824094  1.1414453 18.05531 3.497221  NA        NA
## 3  3.5169528 0.154365 17.677665  5.6633481 32.01948 3.267103  NA        NA
## 4  6.7882463 0.289420 30.531235 10.1852510 45.98364 3.036985   3 -31.51000
## 5  6.5609982 0.190640 32.492465  0.2430544 41.28052 0.853382   3 -31.66333
## 6  8.0026500 0.262090 68.516860  0.6978517 69.92417 1.839787  NA        NA
##    SD.d13C N_d13C.diss MES.mg.L MES.sd MO.mg.L Conc.Solids.mug.gMES
## 1       NA          NA       NA     NA      NA             0.6447290
## 2       NA          NA 53.44444     NA   0e+00             0.6447290
## 3       NA          NA       NA     NA      NA             0.3853094
## 4 0.1039230           3 62.50000     NA   1e-03             0.1258897
## 5 0.1517674           3 22.50000     NA   1e-04             0.4357872
## 6       NA          NA       NA     NA      NA             0.2575699
##   Conc.Solids.ug.gMES.SD N.y filt.d13C filt.SD.d13C DD13C.diss DD13C.filt
## 1             0.02323755  NA        NA           NA         NA         NA
## 2             0.02323755  NA        NA           NA         NA         NA
## 3             0.02515062  NA        NA           NA         NA         NA
## 4             0.02706369  NA        NA           NA  0.7400000         NA
```

```
## 5             0.12323706  NA        NA           NA  0.5866667         NA
## 6             0.06396039  NA        NA           NA         NA         NA
##   NH4.mM TIC.ppm.filt   Cl.mM NO3...mM PO4..mM NPOC.ppm TIC.ppm.unfilt
## 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   0.05         51.8    1.48      616      NA      4.0           44.8
## 5     NA         44.8 1574.00      778      NA      4.4           26.4
## 6     NA           NA      NA       NA      NA       NA             NA
##   TOC.ppm.unfilt ExpMES.Kg Appl.Mass.g Appl.Mass.g.OT Appl.Mass.g.N
## 1             NA  5.352733    31670.07       24477.49      8429.434
## 2             NA  5.352733        0.00           0.00         0.000
## 3             NA 14.875343        0.00           0.00         0.000
## 4            4.7 24.397953        0.00           0.00         0.000
## 5            5.4  8.083000        0.00           0.00         0.000
## 6             NA  7.935755        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 DissSmeto.mg DissSmeto.mg.SD DissSmeto.g
## 1          13320.74     3.541705       0.2783949 0.003541705
## 2          13320.74    24.604033       1.9339946 0.024604033
```

```
## 3          13320.74   170.038598       7.4632812 0.170038598
## 4          13320.74  2649.909084     112.9800910 2.649909084
## 5          13320.74  2357.002211      68.4863626 2.357002211
## 6          13320.74  7021.341115     229.9517390 7.021341115
##   DissSmeto.g.SD  DissOXA.mg DissOXA.mg.SD   DissOXA.g DissOXA.g.SD
## 1   0.0002783949    69.54963      16.45637  0.06954963   0.01645637
## 2   0.0019339946   483.15756     114.32155  0.48315756   0.11432155
## 3   0.0074632812   854.68456     273.81310  0.85468456   0.27381310
## 4   0.1129800910 11918.39439    3975.98846 11.91839439   3.97598846
## 5   0.0684863626 11672.73795      87.31596 11.67273795   0.08731596
## 6   0.2299517390 60115.11746     612.27900 60.11511746   0.61227900
##   DissESA.mg DissESA.mg.SD  DissESA.g DissESA.g.SD FiltSmeto.mg
## 1   260.3058      50.41991  0.2603058   0.05041991     3.451062
## 2  1808.3308     350.26441  1.8083308   0.35026441     3.451062
## 3  1548.0863     157.95877  1.5480863   0.15795877     5.731609
## 4 17950.5083    1185.53932 17.9505083   1.18553932     3.071452
## 5 14829.7964     306.57276 14.8297964   0.30657276     3.522468
## 6 61349.8588    1614.18699 61.3498588   1.61418699     2.044012
##   FiltSmeto.mg.SD FiltSmeto.g FiltSmeto.g.SD TotSMout.mg TotSMout.mg.SD
## 1       0.1243844 0.003451062   0.0001243844    6.992766      0.2156098
## 2       0.1243844 0.003451062   0.0001243844   28.055095      1.3703661
## 3       0.3741240 0.005731609   0.0003741240  175.770206      5.2839633
## 4       0.6602985 0.003071452   0.0006602985 2652.980536     79.8903528
## 5       0.9961252 0.003522468   0.0009961252 2360.524679     48.4322936
## 6       0.5075740 0.002044012   0.0005075740 7023.385126    162.6008301
##    TotSMout.g TotSMout.g.SD  FracDiss     FracFilt     MELsm.g MELsm.g.SD
## 1 0.006992766  0.0002156098 0.5064812 0.4935188249   0.3021264 0.02689497
## 2 0.028055095  0.0013703661 0.8769898 0.1230101642   2.0783329 0.18683762
## 3 0.175770206  0.0052839633 0.9673915 0.0326085349   2.3790960 0.17885971
## 4 2.652980536  0.0798903528 0.9988423 0.0011577363  30.2413655 2.40621294
## 5 2.360524679  0.0484322936 0.9985078 0.0014922393  27.0082117 0.16340841
## 6 7.023385126  0.1626008301 0.9997090 0.0002910294 121.0040582 0.88525127
##   CumOutDiss.g CumOutFilt.g CumOutSmeto.g CumOutMELsm.g BalMassDisch.g
## 1  0.003541705  0.003451062   0.006992766     0.3021264       31669.77
## 2  0.028145738  0.006902124   0.035047862     2.3804594       31667.69
## 3  0.198184336  0.012633733   0.210818068     4.7595554       31665.31
## 4  2.848093419  0.015705185   2.863798604    35.0009209       31635.07
## 5  5.205095630  0.019227652   5.224323282    62.0091326       31608.06
## 6 12.226436745  0.021271664  12.247708409   183.0131909       31487.06
##    prctMassOut FracDeltaOut Events Weeks Event
## 1 4.980859e-05    0.0000000    0-1    W0     0
## 2 1.998329e-04    0.0000000    0-2    W0     0
## 3 1.251989e-03    0.0000000    0-3    W0     0
## 4 1.889684e-02   -0.5954396    1-1    W1     1
## 5 1.681372e-02   -0.5323784    1-2    W1     1
## 6 5.002668e-02    0.0000000    1-3    W1     1
```

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

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