

# 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")
```

```
## 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 #  $\hat{A} \pm 0.4$ 

# 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 #  $\hat{A} \pm 0.33$ 
```

## 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
##   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>
```

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 were 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 "A0-W11-1-1_.dxf",...: 13 14 15 16 17 18 52 53 54 64 ..
## $ ID                   : Factor w/ 1 level "A0": 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/MESAteck_FilterIsotopes.csv", header = T, dec = ".")
#filtersIso <- filtersIso[filtersIso$Levl != "J+7", ]
if (length(filtersIso) == 1){
  filtersIso = read.csv("Data/MESAteck_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/A0-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 steps

1. Merge all data sets by the *WeekSubWeek* column ID, including:

```

# 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)

# Hydrochemistry
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

# Temporarily remove Weeks 16 & 17 (need to get discharge data)
# No discharge data yet available 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/106 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)

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 57 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
## $ dryHrsIni : num 0.0333 0.1167 4.2167
## $ dryHrsMax : num 24.52 4.2 5.43
## $ dryHrsAve : num 7.83 1.29 1.31
## $ noEventHrsIni : num 6.02 66.13 1.65
## $ noEventHrsMax : num 47.28 72.1 6.37
## $ noEventHrsAve : num 26.65 30.4 3.33
## $ 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
## $ CumRain.mm : num 7.6 16.8 6
## $ RainInt.mmhr : num 0.0921 0.6161 0.2594
## $ 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  $A_{tr}$  (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 Corn, not Beet

### 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, Friess 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 applications
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.Mathis*(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.NoSo']
  }
}

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 (Continuous)
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:

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

```

# 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. [ $\mu\text{g s-meto/L H}_2\text{O}$ ] * Vol[m3] * [ $10^{-3}$  L/m3] * [1 mg/ $10^{-3}$   $\mu\text{g}$ ]
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. [ $\mu\text{g s-meto / g MES}$ ] * Kg MES * [ $10^{-3}$  g/Kg] * [1 mg/ $10^{-3}$   $\mu\text{g}$ ]
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.SD2 +

```



```

      (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:

```

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

## SM mass sampled: 91.10687

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

## SM mass sampled and non-sampled: 140.392784355072

# Cumulative 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)
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	53.444444	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	
##	P04..mM	NPOC.ppm	TIC.ppm.unfilt	TOC.ppm.unfilt	ExpMES.Kg	Appl.Mass.g		
## 1	NA	NA	NA	NA	5.352733	31670.07		
## 2	NA	NA	NA	NA	5.352733	0.00		
## 3	NA	NA	NA	NA	14.875343	0.00		
## 4	NA	4.0	44.8	4.7	24.397953	0.00		
## 5	NA	4.4	26.4	5.4	8.083000	0.00		
## 6	NA	NA	NA	NA	7.935755	0.00		
##	Appl.Mass.g.OT	Appl.Mass.g.N	Appl.Mass.g.T	Appl.Mass.g.S				
## 1	24477.49	8429.434	6903.61	16337.03				
## 2	0.00	0.000	0.00	0.00				
## 3	0.00	0.000	0.00	0.00				
## 4	0.00	0.000	0.00	0.00				
## 5	0.00	0.000	0.00	0.00				
## 6	0.00	0.000	0.00	0.00				
##	Appl.Mass.g.N.OT	Appl.Mass.g.T.OT	Appl.Mass.g.S.OT	iniCo.ug.g.N				
## 1	8429.434	2727.322	13320.74	8.455948				
## 2	0.000	0.000	0.00	8.455948				

## 3	0.000	0.000	0.00	8.455948	
## 4	0.000	0.000	0.00	8.455948	
## 5	0.000	0.000	0.00	8.455948	
## 6	0.000	0.000	0.00	8.455948	
##	iniCo.ug.g.T	iniCo.ug.g.S	timeSinceApp	timeSinceApp.N	timeSinceApp.T
## 1	7.090939	12.36774	0.5	0.5	0.5
## 2	7.090939	12.36774	3.9	3.9	3.9
## 3	7.090939	12.36774	5.5	5.5	5.5
## 4	7.090939	12.36774	6.6	6.6	6.6
## 5	7.090939	12.36774	7.6	7.6	7.6
## 6	7.090939	12.36774	11.6	11.6	11.6
##	timeSinceApp.S	Appl.Mass.g.NoSo	timeSinceApp.NoSo	CumAppMass.g	
## 1	0.5	31670.07	0.5	31670.07	
## 2	3.9	0.00	3.9	31670.07	
## 3	5.5	0.00	5.5	31670.07	
## 4	6.6	0.00	6.6	31670.07	
## 5	7.6	0.00	7.6	31670.07	
## 6	11.6	0.00	11.6	31670.07	
##	CumAppMass.g.OT	CumAppMass.g.N	CumAppMass.g.T	CumAppMass.g.S	
## 1	24477.49	8429.434	6903.61	16337.03	
## 2	24477.49	8429.434	6903.61	16337.03	
## 3	24477.49	8429.434	6903.61	16337.03	
## 4	24477.49	8429.434	6903.61	16337.03	
## 5	24477.49	8429.434	6903.61	16337.03	
## 6	24477.49	8429.434	6903.61	16337.03	
##	CumAppMass.g.N.OT	CumAppMass.g.T.OT	CumAppMass.g.S.OT	DissSmeto.mg	
## 1	8429.434	2727.322	13320.74	3.541705	
## 2	8429.434	2727.322	13320.74	24.604033	
## 3	8429.434	2727.322	13320.74	170.038598	
## 4	8429.434	2727.322	13320.74	2649.909084	
## 5	8429.434	2727.322	13320.74	2357.002211	
## 6	8429.434	2727.322	13320.74	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 BalMassDisch.g prctMassOut FracDeltaOut
## 1 0.006992766      0.3021264      31669.77 4.980859e-05 0.0000000
## 2 0.035047862      2.3804594      31667.69 1.998329e-04 0.0000000
## 3 0.210818068      4.7595554      31665.31 1.251989e-03 0.0000000
## 4 2.863798604     35.0009209      31635.07 1.889684e-02 -0.5954396
## 5 5.224323282     62.0091326      31608.06 1.681372e-02 -0.5323784
## 6 12.247708409    183.0131909      31487.06 5.002668e-02 0.0000000
##      Events Weeks Event
## 1    0-1      W0      0
## 2    0-2      W0      0
## 3    0-3      W0      0
## 4    1-1      W1      1
## 5    1-2      W1      1
## 6    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")
```