# 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 the weekly discharge summary and lab results for isotopes ($^{13}C$) and s-metolachlor concentrations.

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")
```

## 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"
```

## 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      peak    valley    tdiff  chExtreme
## 1 -0.1193728  1.248600  1.118296 11.96667 -0.1303036
## 2  0.1887431  1.380388  1.082199 82.53333  0.2560062
## 3  0.1482496  1.637782  0.929055 37.63333  0.3296817
## 4 14.9893566 38.399790  1.448977 27.26667 36.9437102
## 5 -1.1498131 18.668972 13.201113 23.13333 -3.1332355
## 6 -9.3472489 15.895640  5.471042 96.33333 -9.7325862
```

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
```

```
# 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)
head(outletIso)
```

```
##   FileHeader..Filename ID Week Wnum SubWeek WeekSubWeek Repl d.13C.12C
## 1        AO_W0_1-1.dxf AO   W0    0       1        W0-1    1   -26.035
## 2        AO_W0_1-2.dxf AO   W0    0       1        W0-1    2   -27.740
## 3  AO_W0_1-3_-0001.dxf AO   W0    0       1        W0-1    3   -26.219
## 4       AO_W2_2-1_.dxf AO   W2    2       2        W2-2    1   -28.609
## 5       AO_W2_2-2_.dxf AO   W2    2       2        W2-2    2   -28.894
## 6       AO_W2_2-3_.dxf AO   W2    2       2        W2-2    3   -28.503
##   DD13...31.21. Ave...STDEV     Rt Ampl..44 Std.Ampl.    ng..C.
## 1         5.175   0.9357993 2651.2      239       858  8.356643
## 2         3.470          NA 2649.3      296       858 10.349650
## 3         4.991          NA 2649.7      302       858 10.559441
## 4         2.601   0.2022136 2656.2      127       658  5.790274
## 5         2.316          NA 2656.2      163       658  7.431611
## 6         2.707          NA 2655.3      176       658  8.024316
```

```
colnames(outletIso)[colnames(outletIso) == "DD13...31.21."] <- "DD13"
colnames(outletIso)[colnames(outletIso) == "ng..C."] <- "ngC"
outletIso <- subset(outletIso, DD13 > 0 & DD13 < 10 & ngC >= 2)

# Filter isotope data:
filtersIso = read.csv2("Data/MESAlteck_FilterIsotopes.csv", header = T)
filtersIso$WeekSubWeek = paste(filtersIso$Week, filtersIso$Num, sep = "-")
filtersIso <- filtersIso[filtersIso$Levl != "J+7", ]
head(filtersIso)
```

```
##    ID Week Wnum Num Levl Repl d.13C.12C WeekSubWeek
## 1 AFP   W2    1   1    1    1   -25.154        W2-1
## 2 AFP   W2    1   1    2    2   -28.187        W2-1
## 3 AFP   W2    1   1    3    3   -28.283        W2-1
## 4 AFP   W2    2   2    1    1   -30.618        W2-2
## 5 AFP   W2    2   2    2    2   -26.304        W2-2
## 6 AFP   W2    2   2    3    3   -26.024        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

```
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))

head(isoOutSummary)
```

```
##   WeekSubWeek N diss.d13C   SD.d13C    se.d13C
## 1        W0-1 3 -26.66467 0.9357993 0.54028398
## 2        W1-1 3 -30.46867 0.1060016 0.06120004
## 3        W1-2 3 -30.61967 0.1513550 0.08738484
## 4       W10-1 2 -29.47350 1.9905056 1.40750000
## 5       W10-2 3 -29.27067 0.6003202 0.34659502
## 6       W10-3 3 -29.76967 0.3411749 0.19697744
```

```
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))
head(isoFiltSummary)
```

```
##   WeekSubWeek N filt.d13C filt.SD.d13C filt.se.d13C
## 1        W2-1 3 -27.20800     1.779464    1.0273738
## 2        W2-2 3 -27.64867     2.575326    1.4868653
## 3        W6-3 3 -28.00667     1.593462    0.9199856
## 4        W9-1 2 -26.79150     1.745847    1.2345000
## 5        W9-2 3 -27.69633     2.013989    1.1627772
## 6        W9-3 3 -26.94633     1.685361    0.9730434
```

## 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)

# Pure and cuve isotope average
d13Co = -31.21

# 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

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

out.CoIs$f.diss <- (((10**(-3)*out.CoIs$diss.d13C + 1)/(10**(-3)*d13Co + 1))**(1000/(epsilon_mean)))
out.CoIs$f.filt <- (((10**(-3)*out.CoIs$filt.d13C + 1)/(10**(-3)*d13Co + 1))**(1000/(epsilon_mean)))

out.CoIs$B.diss <- (1 - out.CoIs$f.diss)*100
out.CoIs$B.filt <- (1 - out.CoIs$f.filt)*100
#out.CoIs$invf <- 1/out.CoIs$f

# 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
```

3. Weekly exported S-metolachlor mass (mg)

```
# 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

# 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

# Total
out.CoIs$TotMassOut.mg = out.CoIs$DissSmeto.mg + out.CoIs$FiltSmeto.mg


# Proportion in dissolved and suspended solids
out.CoIs$FracDiss = out.CoIs$DissSmeto.mg/out.CoIs$TotMassOut.mg
out.CoIs$FracFilt = out.CoIs$FiltSmeto.mg/out.CoIs$TotMassOut.mg
```

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

The five application dates were:

- 2016-03-20
- 2016-04-05
- 2016-04-13 and 2016-04-14
- 2016-05-26

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('2016-05-31 12:00:00' , tz="EST"))

Appl.Mass.g = c(6369.396, 3128.475, 4744.571, 4982.038)

applics = as.data.frame(ti)
applics$Appl.Mass.g = Appl.Mass.g

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)

# Cumulative (Continous)
out.CoIs$CumAppMass.g = cumsum(out.CoIs$Appl.Mass.g)
```

## Section to UPDATE!!!

5. This section converts the observed S-metolachlor concentrations to [g] in dissolved water and suspended solids, assuming 0 for the values where no sample was taken. An approximative model will be tested at a later stage.

```
# First simulate a mass out to deal with missing values
# Option 1, just assume 0.0
out.CoIs$SimOutDiss.g = out.CoIs$DissSmeto.mg/10^3
out.CoIs$SimOutFilt.g = out.CoIs$FiltSmeto.mg/10^3
out.CoIs$SimOutDiss.g = ifelse(is.na(out.CoIs$SimOutDiss.g), 0.0, out.CoIs$SimOutDiss.g)
out.CoIs$SimOutFilt.g = ifelse(is.na(out.CoIs$SimOutFilt.g), 0.0, out.CoIs$SimOutFilt.g)
```

```
out.CoIs$SimOutSmeto.g = out.CoIs$SimOutDiss.g + out.CoIs$SimOutFilt.g

# Cumulative OUT
out.CoIs$CumOutDiss.g = cumsum(out.CoIs$SimOutDiss.g)
out.CoIs$CumOutFilt.g = cumsum(out.CoIs$SimOutFilt.g)
out.CoIs$CumOutSmeto.g = out.CoIs$CumOutDiss.g + out.CoIs$CumOutFilt.g

# Balance
out.CoIs$BalMassDisch.g = out.CoIs$CumAppMass.g - out.CoIs$CumOutSmeto.g

# Mass fraction
massOUT = tail(out.CoIs$CumOutSmeto.g, n=1)
out.CoIs$FracMassOut = (out.CoIs$SimOutSmeto.g / massOUT)
out.CoIs$FracDeltaOut = (out.CoIs$SimOutSmeto.g / massOUT)*out.CoIs$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
massOUT
```

```
## [1] 91.10687
```

```
# Bulk isotope signature
BulkDeltaOut
```

```
## [1] -28.12241
```

6. Testing a regression tree (ommitted for now)

## Save files

```
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      peak    valley    tdiff  chExtreme AveDischarge.m3.h
## 1 -0.1193728  1.248600  1.118296 11.96667 -0.1303036          1.204775
## 2  0.1887431  1.380388  1.082199 82.53333  0.2560062          1.213511
## 3  0.1482496  1.637782  0.929055 37.63333  0.3296817          1.284719
## 4 14.9893566 38.399790  1.448977 27.26667 36.9437102         14.316647
## 5 -1.1498131 18.668972 13.201113 23.13333 -3.1332355         15.529299
## 6 -9.3472489 15.895640  5.471042 96.33333 -9.7325862          9.107720
##   Volume.m3 Sampled.Hrs     Sampled Conc.mug.L Conc.SD  OXA_mean
## 1  14.41714    11.96667 Not Sampled         NA      NA        NA
## 2 100.15508    82.53333     Sampled  0.2456594 0.01931  4.824094
## 3  48.34827    37.63333 Not Sampled         NA      NA        NA
## 4 390.36726    27.26667     Sampled  6.7882463 0.28942 30.531235
```

```
## 5 359.24445    23.13333     Sampled  6.5609982 0.19064 32.492465
## 6 877.37700    96.33333 Not Sampled         NA      NA        NA
##       OXA_SD ESA_mean   ESA_SD N.x diss.d13C   SD.d13C    se.d13C MES.mg.L
## 1         NA       NA       NA  NA        NA        NA         NA       NA
## 2  1.1414453 18.05531 3.497221   3 -26.66467 0.9357993 0.54028398 53.44444
## 3         NA       NA       NA  NA        NA        NA         NA       NA
## 4 10.1852510 45.98364 3.036985   3 -30.46867 0.1060016 0.06120004 62.50000
## 5  0.2430544 41.28052 0.853382   3 -30.61967 0.1513550 0.08738484 22.50000
## 6         NA       NA       NA  NA        NA        NA         NA       NA
##   MES.sd MO.mg.L Conc.Solids.mug.gMES N.y filt.d13C filt.SD.d13C
## 1     NA      NA                   NA  NA        NA           NA
## 2     NA   0e+00            0.6447290  NA        NA           NA
## 3     NA      NA                   NA  NA        NA           NA
## 4     NA   1e-03            0.1258897  NA        NA           NA
## 5     NA   1e-04            0.4357872  NA        NA           NA
## 6     NA      NA                   NA  NA        NA           NA
##   filt.se.d13C DD13C.diss DD13C.filt     f.diss f.filt   B.diss B.filt
## 1           NA         NA         NA         NA     NA       NA     NA
## 2           NA  4.5453333         NA 0.06892489     NA 93.10751     NA
## 3           NA         NA         NA         NA     NA       NA     NA
## 4           NA  0.7413333         NA 0.64590754     NA 35.40925     NA
## 5           NA  0.5903333         NA 0.70603206     NA 29.39679     NA
## 6           NA         NA         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 DissSmeto.mg FiltSmeto.mg TotMassOut.mg
## 1             NA        NA           NA           NA            NA
## 2             NA  5.352733     24.60403     3.451062       28.0551
## 3             NA        NA           NA           NA            NA
## 4            4.7 24.397953   2649.90908     3.071452     2652.9805
## 5            5.4  8.083000   2357.00221     3.522468     2360.5247
## 6             NA        NA           NA           NA            NA
##    FracDiss    FracFilt Appl.Mass.g CumAppMass.g SimOutDiss.g SimOutFilt.g
## 1        NA          NA    6369.396     6369.396   0.00000000  0.000000000
## 2 0.8769898 0.123010164       0.000     6369.396   0.02460403  0.003451062
## 3        NA          NA       0.000     6369.396   0.00000000  0.000000000
## 4 0.9988423 0.001157736       0.000     6369.396   2.64990908  0.003071452
## 5 0.9985078 0.001492239       0.000     6369.396   2.35700221  0.003522468
## 6        NA          NA       0.000     6369.396   0.00000000  0.000000000
##   SimOutSmeto.g CumOutDiss.g CumOutFilt.g CumOutSmeto.g BalMassDisch.g
## 1     0.0000000   0.00000000  0.000000000     0.0000000       6369.396
## 2     0.0280551   0.02460403  0.003451062     0.0280551       6369.368
## 3     0.0000000   0.02460403  0.003451062     0.0280551       6369.368
## 4     2.6529805   2.67451312  0.006522514     2.6810356       6366.715
## 5     2.3605247   5.03151533  0.010044982     5.0415603       6364.354
## 6     0.0000000   5.03151533  0.010044982     5.0415603       6364.354
##    FracMassOut FracDeltaOut
## 1 0.0000000000  0.000000000
## 2 0.0003079361 -0.008211013
```

```
## 3 0.0000000000  0.000000000
## 4 0.0291194331 -0.887230300
## 5 0.0259094025 -0.793337267
## 6 0.0000000000  0.000000000
```

```r
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")
```