

# Soils & Discharge Merged

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## Purpose

This file merges outlet data with soil data to plot cumulative exported and remaining S-metolachlor mass. The nearest soil sample date for each transect is used to match the initial time (“ti”) of the sampling discharge period. This is most adequate merging location given that samples took place shortly before relaunching the automatic sampler.

Note that week numbers for water and soils are offset by one. I.e. Week 1 soils influence/regulate Week 2’s water sample results.

Imports:

- WeeklyHydroContam\_R.csv
- WeeklySoils\_R.csv

Generates:

- WeekSoilHydroCont\_R.csv

## Required R-packages:

```
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"
```

## Import files

```
outlet = read.csv2("Data/WeeklyHydroContam_R.csv", header = T)
outlet$ti <- as.POSIXct(outlet$ti, "%Y-%m-%d %H:%M", tz = "EST")
sum(is.na(outlet$ti))
```

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

```
# Select variables from Water dataset
```

```
outlet <- outlet[, c("ti", "WeekSubWeek", "B.diss", "B.filt", "CumOutDiss.g", "CumOutFilt.g", "CumAppMa
print("Water")
```

```
## [1] "Water"
```

```

str(outlet)

## 'data.frame':   51 obs. of  7 variables:
## $ ti           : POSIXct, format: "2016-03-25 00:04:00" "2016-03-25 12:04:00" ...
## $ WeekSubWeek  : Factor w/ 51 levels "W0-0x","W0-1",...: 1 2 3 4 5 6 26 27 28 29 ...
## $ B.diss       : num  NA 93.1 NA 35.4 29.4 ...
## $ B.filt       : num  NA NA NA NA NA ...
## $ CumOutDiss.g: num  0 0.0246 0.0246 2.6745 5.0315 ...
## $ CumOutFilt.g: num  0 0.00345 0.00345 0.00652 0.01004 ...
## $ CumAppMass.g: num  6369 6369 6369 6369 6369 ...

soils = read.csv2("Data/WeeklySoils_Rng.csv", header =T) # Corrected with only ngC > 2.0
soils$Date.ti <- as.POSIXct(soils$Date.ti, "%Y-%m-%d %H:%M", tz = "EST")
#soils$Date.ti <- as.POSIXct(soils$Date.ti, "%d/%m/%Y %H:%M", tz = "EST")
sum(is.na(soils$Date.ti))

## [1] 0

print("Soils")

## [1] "Soils"

str(soils)

## 'data.frame':   51 obs. of  19 variables:
## $ ID           : Factor w/ 51 levels "AW-N-0","AW-N-0x",...: 2 19 36 1 18 35 3 20 37 10 ...
## $ Transect     : Factor w/ 3 levels "N","S","T": 1 2 3 1 2 3 1 2 3 1 ...
## $ Wnum         : int   -1 -1 -1 0 0 0 1 1 1 2 ...
## $ Date.Soil    : Factor w/ 17 levels "03/05/2016 13:10",...: 13 13 13 16 16 16 3 3 3 7 ...
## $ Date.ti      : POSIXct, format: "2016-03-25 00:04:00" "2016-03-25 00:04:00" ...
## $ Conc.mug.g.dry.soil: num  0.018 0.029 0.02 1.398 2.881 ...
## $ Conc.ComSoil.SD : num  NA NA NA NA NA ...
## $ N_compsoil    : int   NA NA NA NA NA NA 2 2 3 3 ...
## $ comp.d13C     : num  NA NA NA NA NA ...
## $ comp.d13C.SD  : num  NA NA NA NA NA ...
## $ comp.d13C.SE  : num  NA NA NA NA NA ...
## $ DD13C.comp    : num  NA NA NA NA NA ...
## $ f.comp        : num  NA NA NA NA NA ...
## $ B.comp        : num  NA NA NA NA NA ...
## $ f.min.comp    : num  NA NA NA NA NA ...
## $ B.min.comp    : num  NA NA NA NA NA ...
## $ f.mean.comp   : num  NA NA NA NA NA ...
## $ B.mean.com    : num  NA NA NA NA NA ...
## $ MassSoil.g    : num  12.41 15.87 6.49 963.74 1576.37 ...

```

Get soil concentrations for each transect for merging horizontally

```

# North
soils.N <- subset(soils, soils$Transect == "N")
soils.N <- soils.N[, c("Date.ti", "B.comp", "MassSoil.g", "comp.d13C", "comp.d13C.SD", "comp.d13C.SE", "
colnames(soils.N) <- c("ti", "B.comp.North", "MassSoil.g.North", "comp.d13C.North", "comp.d13C.SD.North", "comp.d13C.SE.North")

# Talweg
soils.T <- subset(soils, soils$Transect == "T")

```

```

soils.T <- soils.T[, c("Date.ti", "B.comp", "MassSoil.g", "comp.d13C", "comp.d13C.SD", "comp.d13C.SE", "
colnames(soils.T) <- c("ti", "B.comp.Talweg", "MassSoil.g.Talweg", "comp.d13C.Talweg", "comp.d13C.SD.T

# South
soils.S <- subset(soils, soils$Transect == "S")
soils.S <- soils.S[, c("Date.ti", "B.comp", "MassSoil.g", "comp.d13C", "comp.d13C.SD", "comp.d13C.SE", "
colnames(soils.S) <- c("ti", "B.comp.South", "MassSoil.g.South", "comp.d13C.South", "comp.d13C.SD.South")

```

## Total Catchment Mass and Bulk Isotopes

Bulk isotopes are calculated based on the following:

$$\delta_{bulk} = \frac{M_{North}}{M_{tot}}\delta_{North} + \frac{M_{Talweg}}{M_{tot}}\delta_{Talweg} + \frac{M_{South}}{M_{tot}}\delta_{South}$$

```

library(zoo)

##
## Attaching package: 'zoo'

## The following objects are masked from 'package:base':
##
##      as.Date, as.Date.numeric

class(outlet$ti)

## [1] "POSIXct" "POSIXt"

class(soils.T$ti)

## [1] "POSIXct" "POSIXt"

soilsOut <- merge(outlet, soils.N, by = "ti", all = T)
soilsOut <- merge(soilsOut, soils.T, by = "ti", all = T)
soilsOut <- merge(soilsOut, soils.S, by = "ti", all = T)

# Total mass in catchment
soilsOut$CatchMassSoil.g <- soilsOut$MassSoil.g.North + soilsOut$MassSoil.g.Talweg + soilsOut$MassSoil.g.South

# Bulk catchment isotopes
soilsOut$BulkCatch.d13 <-
  (soilsOut$MassSoil.g.North/soilsOut$CatchMassSoil.g)*soilsOut$comp.d13C.North +
  (soilsOut$MassSoil.g.Talweg/soilsOut$CatchMassSoil.g)*soilsOut$comp.d13C.Talweg +
  (soilsOut$MassSoil.g.South/soilsOut$CatchMassSoil.g)*soilsOut$comp.d13C.South

print("Merged Soils and Outlet by ti")

## [1] "Merged Soils and Outlet by ti"

str(soilsOut)

## 'data.frame':   52 obs. of  27 variables:
##  $ ti              : POSIXct, format: "2016-03-25 00:04:00" "2016-03-25 12:04:00" ...
##  $ WeekSubWeek     : Factor w/ 51 levels "W0-0x","W0-1",...: 1 2 3 4 5 6 26 27 28 29 ...
##  $ B.diss          : num  NA 93.1 NA 35.4 29.4 ...
##  $ B.filt          : num  NA NA NA NA NA ...

```

```
## $ CumOutDiss.g      : num  0 0.0246 0.0246 2.6745 5.0315 ...
## $ CumOutFilt.g      : num  0 0.00345 0.00345 0.00652 0.01004 ...
## $ CumAppMass.g      : num  6369 6369 6369 6369 6369 ...
## $ B.comp.North      : num  NA NA NA NA NA ...
## $ MassSoil.g.North  : num  12.4 NA NA 963.7 NA ...
## $ comp.d13C.North   : num  NA NA NA NA NA ...
## $ comp.d13C.SD.North : num  NA NA NA NA NA ...
## $ comp.d13C.SE.North : num  NA NA NA NA NA ...
## $ ID.N              : Factor w/ 51 levels "AW-N-0","AW-N-0x",...: 2 NA NA 1 NA NA 3 NA NA 10 ...
## $ B.comp.Talweg     : num  NA NA NA NA NA ...
## $ MassSoil.g.Talweg : num  6.49 NA NA 365.21 NA ...
## $ comp.d13C.Talweg  : num  NA NA NA NA NA ...
## $ comp.d13C.SD.Talweg: num  NA NA NA NA NA ...
## $ comp.d13C.SE.Talweg: num  NA NA NA NA NA ...
## $ ID.T              : Factor w/ 51 levels "AW-N-0","AW-N-0x",...: 36 NA NA 35 NA NA 37 NA NA 44 ...
## $ B.comp.South      : num  NA NA NA NA NA ...
## $ MassSoil.g.South  : num  15.9 NA NA 1576.4 NA ...
## $ comp.d13C.South   : num  NA NA NA NA NA ...
## $ comp.d13C.SD.South : num  NA NA NA NA NA ...
## $ comp.d13C.SE.South : num  NA NA NA NA NA ...
## $ ID.S              : Factor w/ 51 levels "AW-N-0","AW-N-0x",...: 19 NA NA 18 NA NA 20 NA NA 27 ...
## $ CatchMassSoil.g   : num  34.8 NA NA 2905.3 NA ...
## $ BulkCatch.d13     : num  NA NA NA NA NA ...

write.csv2(soilsOut,
           'Data/MassBalance_R.csv', row.names = F)
```

## Plot

```
library("ggplot2")
library("scales")
library("reshape2")
library("cowplot")

##
## Attaching package: 'cowplot'

## The following object is masked from 'package:ggplot2':
##
##     ggsave

# Melt data set
##Subset the necessary columns
soilsRemainMass <- soilsOut[, c("ti", "CumAppMass.g", "CumOutDiss.g", "CumOutFilt.g", "CatchMassSoil.g")]

# Replace each NA with the most recent non-NA prior to it.
# Purpose: To match continuous outlet time array
soilsRemainMass$CatchMassSoil.g <- na.locf(soilsRemainMass$CatchMassSoil.g)

##Then rearrange your data frame
remainMassMolten = melt(soilsRemainMass, id=c("ti"))
# View(remainMassMolten)
```

```

pg <- remainMassMolten
# Change variable names:
levels(pg$variable)[levels(pg$variable)=="CumAppMass.g"] <- "Applied Cum. (Survey)"
levels(pg$variable)[levels(pg$variable)=="CumOutDiss.g"] <- "Dissolved Cum. (Outlet)"
levels(pg$variable)[levels(pg$variable)=="CumOutFilt.g"] <- "Sediment Cum. (Outlet)"
levels(pg$variable)[levels(pg$variable)=="CatchMassSoil.g"] <- "Catchment Mass (1cm Soil)"

# Change the order:
levels(pg$variable)

## [1] "Applied Cum. (Survey)"      "Dissolved Cum. (Outlet)"
## [3] "Sediment Cum. (Outlet)"    "Catchment Mass (1cm Soil)"

pg$variable <- factor(pg$variable, levels = c("Applied Cum. (Survey)", "Catchment Mass (1cm Soil)", "Dissolved Cum. (Outlet)", "Sediment Cum. (Outlet)"))
# names(pg)[names(pg)=="variable"] <- "Estimated Mass"

massBalTop <- ggplot(pg) +
  geom_line(aes(x=ti, y=value, group = variable, color=variable)) +

  # Themes and axes
  theme_bw() +
  theme(# axis.text.x=element_text(angle = 45, hjust = 1),
        axis.text.x=element_blank(),
        axis.title.x=element_blank(),
        legend.position="top"

        )+
  labs(color = "Estimated Mass") +
  guides(col = guide_legend(ncol = 2)) + # Sets legend parameters

  # xlab("Date") +
  scale_x_datetime(breaks = date_breaks("2 weeks"), labels = date_format("%b %d")) +
  ylab(expression(paste("Mass. S-Meto. ", {(g)}))) # +
  # scale_y_continuous(breaks = c(100, 5000, 10000, 20000), limits = c(100, 20000) )
  # scale_y_continuous(trans=log_trans(), breaks=c(1,5,10,50,100,500,1000,2000,3000,4000,5000))

massBalBottom <- ggplot(pg) +
  geom_line(aes(x=ti, y=value, color=variable)) +

  # Themes and axes
  theme_bw() +
  theme(axis.text.x=element_text(angle = 45, hjust = 1),
        #axis.text.x=element_blank(),
        #axis.title.x=element_blank(),
        legend.position="none"

        )+
  # guides(col = guide_legend(nrows = 2)) + # Sets legend parameters
  xlab("Date") +
  scale_x_datetime(breaks = date_breaks("2 weeks"), labels = date_format("%b %d")) +
  ylab(expression(paste("Mass. S-Meto. ", {(g)}))) +
  scale_y_continuous(breaks = c(1, 25, 50, 100), limits = c(0, 100) )

```

```
massBal = plot_grid(massBalTop, massBalBottom, ncol = 1, nrow = 2, align = "v")
```

```
## Warning: Removed 3 rows containing missing values (geom_path).
```

```
## Warning: Removed 51 rows containing missing values (geom_path).
```

```
massBal
```

