

Soils & Discharge Merged

PAZ

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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  8 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  0.00354 0.02815 0.19818 2.84809 5.2051 ...
## $ CumOutFilt.g     : num  0.00345 0.0069 0.01263 0.01571 0.01923 ...
## $ CumAppMass.g     : num  6369 6369 6369 6369 6369 ...
## $ CumOutMELsm.g    : num  0.302 2.38 4.76 35.001 62.009 ...
```

```
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  26 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 NA NA 2 NA 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 ...
## $ N_ngC            : int   NA NA NA NA NA NA NA NA 2 NA 3 ...
## $ ngC.mean         : num   NA NA NA NA NA ...
## $ ngC.SD           : num   NA NA NA NA NA ...
## $ ngC.SE           : num   NA NA NA NA NA ...
## $ DD13C.comp       : num   NA NA NA NA NA ...
## $ f.max.comp       : num   NA NA NA NA NA ...
## $ B.max.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.comp      : num   NA NA NA NA NA ...
## $ MassSoil.g       : num   12.41 19.12 4.33 963.74 1899.2 ...
## $ Area.N           : num   139266 139266 139266 139266 139266 ...
## $ Area.T           : num   43713 43713 43713 43713 43713 ...
## $ Area.S           : num   133175 133175 133175 133175 133175 ...
```

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.mean.comp", "B.max.comp", "B.min.comp", "MassSoil.g",
                      "comp.d13C", "comp.d13C.SD", "comp.d13C.SE",
                      "ID", "Area.N", "Area.T", "Area.S" )]

colnames(soils.N) <- c("ti", "B.mean.comp.North", "B.max.comp.North", "B.min.comp.North", "MassSoil.g",
                      "comp.d13C.North", "comp.d13C.SD.North", "comp.d13C.SE.North",
                      "ID.N", "Area.N", "Area.T", "Area.S" )

# Talweg
soils.T <- subset(soils, soils$Transect == "T")
soils.T <- soils.T[, c("Date.ti", "B.mean.comp", "B.max.comp", "B.min.comp", "MassSoil.g",
                      "comp.d13C", "comp.d13C.SD", "comp.d13C.SE",
                      "ID")]

colnames(soils.T) <- c("ti", "B.mean.comp.Talweg", "B.max.comp.Talweg", "B.min.comp.Talweg", "MassSoil.g",
                      "comp.d13C.Talweg", "comp.d13C.SD.Talweg", "comp.d13C.SE.Talweg",
                      "ID.T" )

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

colnames(soils.S) <- c("ti", "B.mean.comp.South", "B.max.comp.South", "B.min.comp.South", "MassSoil.g",
                      "comp.d13C.South", "comp.d13C.SD.South", "comp.d13C.SE.South",
                      "ID.S" )
```

Total Catchment Mass, Bulk Mass and Bulk Isotopes

Bulk isotopes are calculated based on the following:

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

Bulk mass is a proxy for the potential mass that can be discharged at a give time. It is calculated base don the pondered mass from each transect area and the proportion of that area in relation to the entire catchment such that:

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

```
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

soilsOut$BulkMass.g <-
  soilsOut$MassSoil.g.North*(soilsOut$Area.N/(soilsOut$Area.N+soilsOut$Area.T+soilsOut$Area.S)) +
  soilsOut$MassSoil.g.Talweg*(soilsOut$Area.T/(soilsOut$Area.N+soilsOut$Area.T+soilsOut$Area.S)) +
  soilsOut$MassSoil.g.South*(soilsOut$Area.S/(soilsOut$Area.N+soilsOut$Area.T+soilsOut$Area.S))

# 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  38 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  0.00354 0.02815 0.19818 2.84809 5.2051 ...
##  $ CumOutFilt.g      : num  0.00345 0.0069 0.01263 0.01571 0.01923 ...
##  $ CumAppMass.g      : num  6369 6369 6369 6369 6369 ...
##  $ CumOutMELsm.g     : num  0.302 2.38 4.76 35.001 62.009 ...
##  $ B.mean.comp.North : num  NA NA NA NA NA ...
##  $ B.max.comp.North  : num  NA NA NA NA NA ...
##  $ B.min.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 ...
##  $ Area.N            : num  139266 NA NA 139266 NA ...
##  $ Area.T            : num  43713 NA NA 43713 NA ...
##  $ Area.S            : num  133175 NA NA 133175 NA ...
##  $ B.mean.comp.Talweg : num  NA NA NA NA NA ...

```

```
## $ B.max.comp.Talweg : num NA NA NA NA NA ...
## $ B.min.comp.Talweg : num NA NA NA NA NA ...
## $ MassSoil.g.Talweg : num 4.33 NA NA 243.43 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.mean.comp.South : num NA NA NA NA NA ...
## $ B.max.comp.South : num NA NA NA NA NA ...
## $ B.min.comp.South : num NA NA NA NA NA ...
## $ MassSoil.g.South : num 19.1 NA NA 1899.2 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 35.9 NA NA 3106.4 NA ...
## $ BulkMass.g : num 14.1 NA NA 1258.2 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", "CumOutMELsm.g"),
```

```
# Replace Catchment Mass's NA with the most recent non-NA prior to it (assumes no degradation).
```

```
# Purpose: To match continuous outlet time array
```

```
soilsRemainMass$CatchMassSoil.g <- na.locf(soilsRemainMass$CatchMassSoil.g)
```

```
soilsRemainMass <- na.omit(soilsRemainMass)
```

```
##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 SM Cum. (Survey)"
levels(pg$variable)[levels(pg$variable)=="CumOutMELsm.g"] <- "MEL-SM Cum. (Outlet)"
levels(pg$variable)[levels(pg$variable)=="CatchMassSoil.g"] <- "Remaining SM (1cm Soil)"

levels(pg$variable)[levels(pg$variable)=="CumOutDiss.g"] <- "Dissolved SM Cum. (Outlet)"
levels(pg$variable)[levels(pg$variable)=="CumOutFilt.g"] <- "Sediment SM Cum. (Outlet)"

# Change the order:
levels(pg$variable)

## [1] "Applied SM Cum. (Survey)"    "Dissolved SM Cum. (Outlet)"
## [3] "Sediment SM Cum. (Outlet)"   "MEL-SM Cum. (Outlet)"
## [5] "Remaining SM (1cm Soil)"

pg$variable <- factor(pg$variable, levels = c("Applied SM Cum. (Survey)", "Remaining SM (1cm Soil)", "Dissolved SM Cum. (Outlet)", "MEL-SM Cum. (Outlet)", "Sediment SM Cum. (Outlet)"))

pgSimple <- pg[which(pg$variable != ("Dissolved SM Cum. (Outlet)") & pg$variable != ("Sediment SM Cum. (Outlet)")), ]
# names(pg)[names(pg)=="variable"] <- "Estimated Mass"

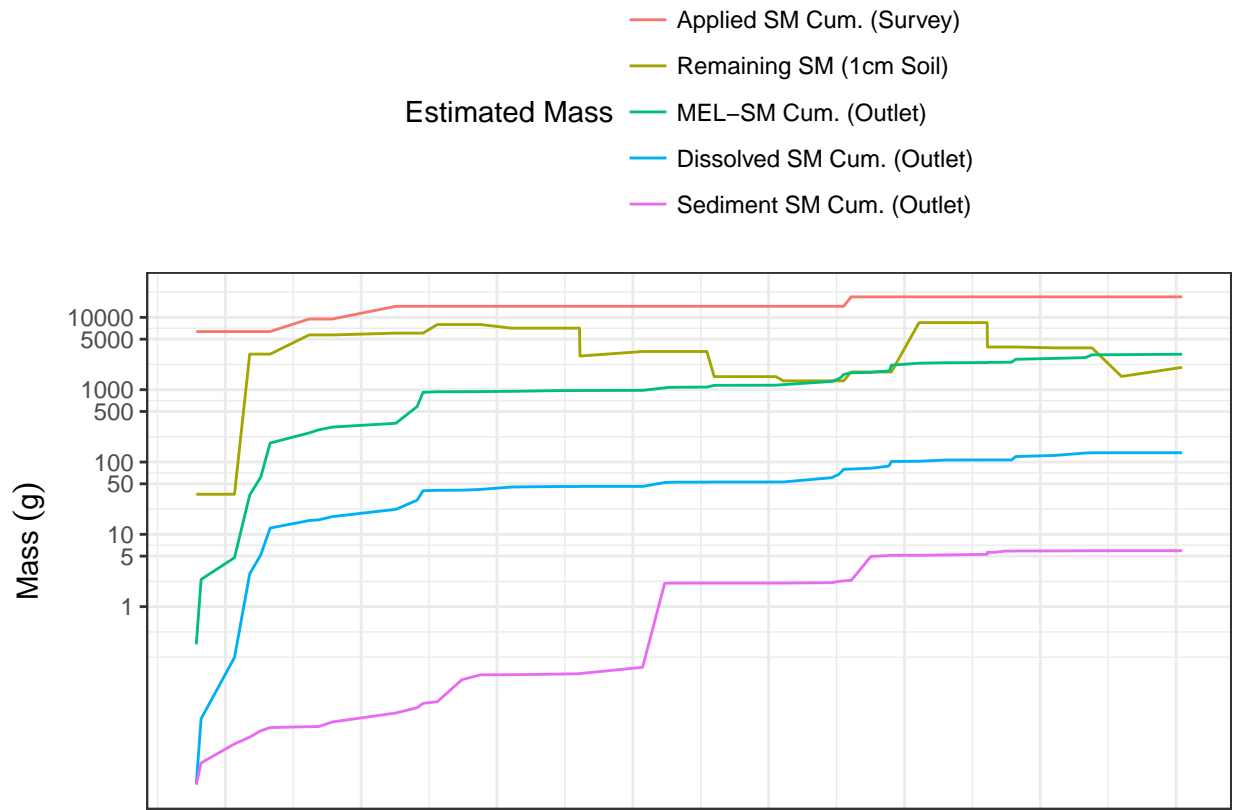
massBalTop <- ggplot(pg) +
  geom_line(aes(x=ti, y=value, group = variable, color=variable)) +

  # 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 = 1)) + # Sets legend parameters

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

```



```
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 108 rows containing missing values (geom_path).
```

```
massBal_MEL <- ggplot(pgSimple) +
  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 = 3)) + # Sets legend parameters

# xlab("Date") +
scale_x_datetime(breaks = date_breaks("2 weeks"), labels = date_format("%b %d")) +
ylab(expression(paste("Mass ", {(g)})))

massBal_MEL

```

