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", "CumAppMas
print("Water")
```

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

```r
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 ...
```

```r
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
```

```r
print("Soils")
```

```
## [1] "Soils"
```

```r
str(soils)
```

```
## 'data.frame':    51 obs. of  22 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 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

```r
# 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",
```

```r
                        "ID", "Area.N", "Area.T", "Area.S" )]

colnames(soils.N) <- c("ti",  "B.comp.North", "MassSoil.g.North",
                        "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.comp", "MassSoil.g",
                        "comp.d13C", "comp.d13C.SD", "comp.d13C.SE",
                        "ID")]

colnames(soils.T) <- c("ti",  "B.comp.Talweg", "MassSoil.g.Talweg",
                        "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.comp", "MassSoil.g",
                        "comp.d13C", "comp.d13C.SD", "comp.d13C.SE",
                        "ID" )]
colnames(soils.S) <- c("ti",  "B.comp.South", "MassSoil.g.South",
                        "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:

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

```r
library(zoo)
```

```
##
## Attaching package: 'zoo'

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

```r
class(outlet$ti)
```

```
## [1] "POSIXct" "POSIXt"
```

```r
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  31 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 ...
##  $ 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.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.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", "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)"
```

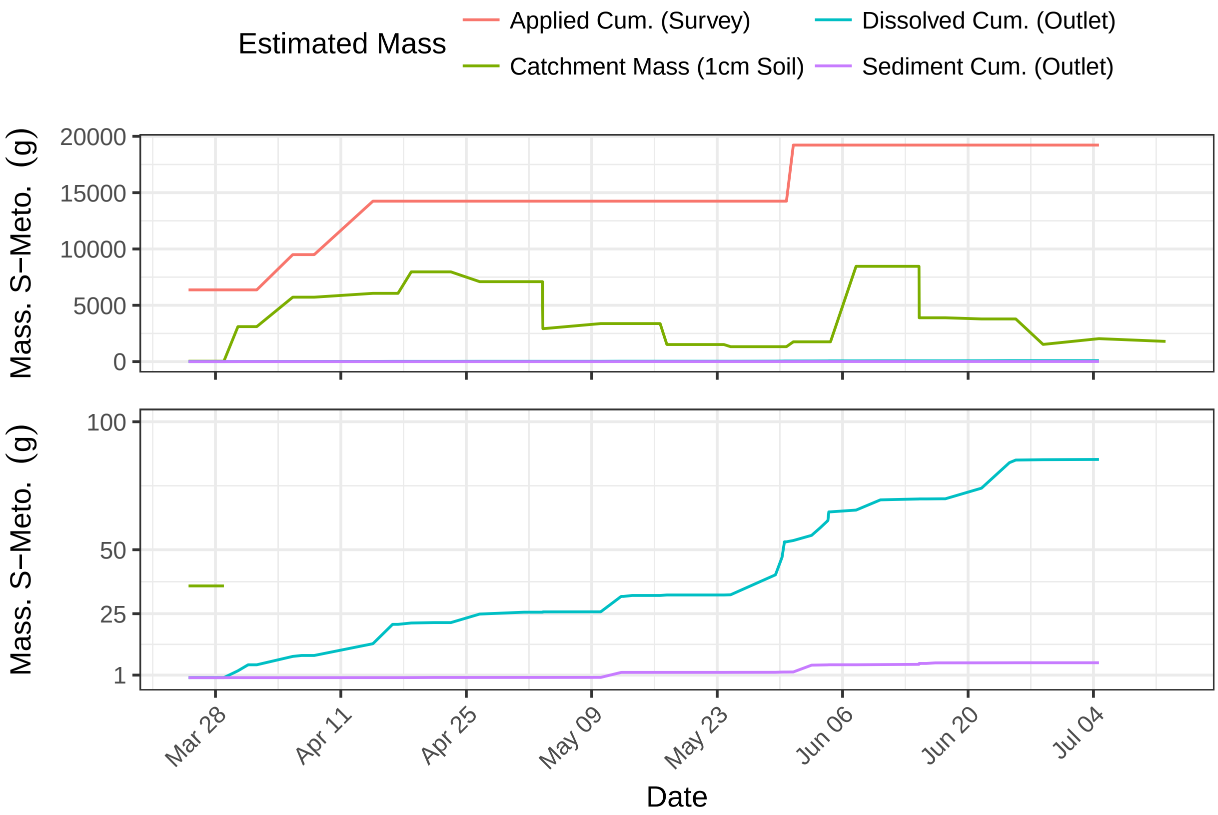
```
pg$variable <- factor(pg$variable, levels = c("Applied Cum. (Survey)", "Catchment Mass (1cm Soil)", "Di
# names(pg)[names(pg)=="variable"]  <- "Estimated Mass"

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
```


Estimated Mass
Applied Cum. (Survey)
Dissolved Cum. (Outlet)
Catchment Mass (1cm Soil)
Sediment Cum. (Outlet)
20000
15000
10000
5000
0
100
50
25
1
Mass. S−Meto. (g)
Mass. S−Meto. (g)
Mar 28
Apr 11
Apr 25
May 09
May 23
Jun 06
Jun 20
Jul 04
Date