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_Rng.csv**

Generates:

- **WeekSoilHydroCont_R.csv**
- **MassBalance_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] "/Users/DayTightChunks/Documents/PhD/HydrologicalMonitoring"
```

Lab Parameters

```
# Pure and cuve isotope average
d13Co = -32.253

# Lab enrichment: Alteck
#epsilon_max = -1.5 # +/- 0.3 (@ 20C, 20% vwc)
#epsilon_min = -2.0 # +/- 0.2 (@ 20C, 40% vwc)

# Ehssan values:
epsilon_max = -1.8
```

```
epsilon_min = -2.6
epsilon_mean = -2.2 # ± 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 # ± 0.33
```

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", "Event", "timeSinceApp", "timeSinceApp.NoSo",
                     "diss.d13C", "SD.d13C",
                     "B.diss", "B.filt", "CumOutDiss.g", "CumOutFilt.g", "CumAppMass.g", "CumOutMELsm.g
print("Water")
```

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

```
str(outlet)
```

```
## 'data.frame':    51 obs. of  13 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 ...
##  $ Event            : int  0 0 0 1 1 1 2 2 2 3 ...
##  $ timeSinceApp     : num  0.5 3.9 5.5 6.6 7.6 11.6 12.6 14 20.6 2.2 ...
##  $ timeSinceApp.NoSo: num  0.5 3.9 5.5 6.6 7.6 11.6 12.6 14 20.6 2.2 ...
##  $ diss.d13C        : num  NA NA NA -31.5 -31.7 ...
##  $ SD.d13C          : num  NA NA NA 0.106 0.151 ...
##  $ B.diss           : num  NA NA NA 29.3 24.1 ...
##  $ 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  17319 17319 17319 17319 17319 ...
##  $ 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  27 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 0.889 3.204 ...
##  $ Conc.ComSoil.SD    : num  NA NA NA 0.133 0.481 ...
##  $ N_compsoil         : int  NA NA NA NA NA NA 3 3 3 3 ...
##  $ comp.d13C          : num  NA NA NA NA NA ...
##  $ comp.d13C.SD       : num  NA NA NA NA NA ...
##  $ N_ngC              : int  NA NA NA NA NA NA 3 3 3 3 ...
##  $ ngC.mean           : num  NA NA NA NA NA ...
##  $ ngC.SD             : num  NA NA NA NA NA ...
##  $ prctError          : num  NA NA NA NA NA ...
##  $ comp.IMP.d13C      : 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  24.82 38.23 8.66 1226.16 4224.23 ...
##  $ MassSoil.g.SD      : num  NA NA NA 184 634 ...
##  $ 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", "MassSoil
                       "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.North", "MassSoil.g.SD.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.mean.comp",  "B.max.comp",  "B.min.comp", "MassSoil.g", "MassSoil.
                       "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.Talweg", "MassSoil.g.SD.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.mean.comp",  "B.max.comp",  "B.min.comp", "MassSoil.g", "MassSoil.
                       "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.South", "MassSoil.g.SD.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 (not currently used) is a proxy for the potential mass that can be discharged at a give time. It is calculated based on 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$CatchMassSoil.g.SD <- (
  ( soilsOut$MassSoil.g.SD.North^2 +
      soilsOut$MassSoil.g.SD.South^2 +
      soilsOut$MassSoil.g.SD.Talweg^2
```

```
    )/3
  )^0.5

# Approximate initial mass for first 6 observation (before recording composite soils)
#soilsOut$CatchMassSoil.g[1:6] <- ifelse(is.na(soilsOut$CatchMassSoil.g),
#                                        soilsOut$CumAppMass.g-soilsOut$CumOutMELsm.g,
#                                        soilsOut$CatchMassSoil.g)


#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

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



# Lab epsilon (mean)
epsilon_mean
```

```
## [1] -2.2
```

```
# Measured initial signature in tank
d13Co
```

```
## [1] -32.253
```

```
soilsOut$BulkCatch.DD13 <-  (soilsOut$BulkCatch.d13 - (d13Co))

# Mean epsilon (# Alteck)
soilsOut$f.mean.bulk <-
  ((10^(-3)*soilsOut$BulkCatch.d13 + 1)/(10^(-3)*d13Co + 1))^(1000/(epsilon_mean))
soilsOut$f.mean.bulk.Field <-
  ((10^(-3)*soilsOut$BulkCatch.d13 + 1)/(10^(-3)*d13Co + 1))^(1000/(epsilonField_mean))

soilsOut$f.min.bulk <-
  ((10^(-3)*soilsOut$BulkCatch.d13 + 1)/(10^(-3)*d13Co + 1))^(1000/(epsilon_max))
soilsOut$f.min.bulk.Field <-
  ((10^(-3)*soilsOut$BulkCatch.d13 + 1)/(10^(-3)*d13Co + 1))^(1000/(epsilonField_max))

soilsOut$f.max.bulk <-
  ((10^(-3)*soilsOut$BulkCatch.d13 + 1)/(10^(-3)*d13Co + 1))^(1000/(epsilon_min))
soilsOut$f.max.bulk.Field <-
  ((10^(-3)*soilsOut$BulkCatch.d13 + 1)/(10^(-3)*d13Co + 1))^(1000/(epsilonField_min))
```

```
soilsOut$B.mean.bulk <-
  (1 - soilsOut$f.mean.bulk)*100
soilsOut$B.min.bulk <-
  (1 - soilsOut$f.max.bulk)*100
soilsOut$B.max.bulk <-
  (1 - soilsOut$f.min.bulk)*100

soilsOut$B.mean.bulk.Field <-
  (1 - soilsOut$f.mean.bulk.Field)*100
soilsOut$B.min.bulk.Field <-
  (1 - soilsOut$f.max.bulk.Field)*100
soilsOut$B.max.bulk.Field <-
  (1 - soilsOut$f.min.bulk.Field)*100

print("Merged Soils and Outlet by ti")
```

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

```
str(soilsOut)
```

```
## 'data.frame':    52 obs. of  57 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 ...
##  $ Event               : int  0 0 0 1 1 1 2 2 2 3 ...
##  $ timeSinceApp        : num  0.5 3.9 5.5 6.6 7.6 11.6 12.6 14 20.6 2.2 ...
##  $ timeSinceApp.NoSo   : num  0.5 3.9 5.5 6.6 7.6 11.6 12.6 14 20.6 2.2 ...
##  $ diss.d13C           : num  NA NA NA -31.5 -31.7 ...
##  $ SD.d13C             : num  NA NA NA 0.106 0.151 ...
##  $ B.diss              : num  NA NA NA 29.3 24.1 ...
##  $ 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  17319 17319 17319 17319 17319 ...
##  $ 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  24.8 NA NA 1226.2 NA ...
##  $ MassSoil.g.SD.North : num  NA NA NA 184 NA ...
##  $ comp.d13C.North     : num  NA NA NA NA NA ...
##  $ comp.d13C.SD.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  8.66 NA NA 346.54 NA ...
##  $ MassSoil.g.SD.Talweg: num  NA NA NA 52 NA ...
##  $ comp.d13C.Talweg    : num  NA NA NA NA NA ...
##  $ comp.d13C.SD.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  38.2 NA NA 4224.2 NA ...
##  $ MassSoil.g.SD.South : num  NA NA NA 634 NA ...
##  $ comp.d13C.South     : num  NA NA NA NA NA ...
##  $ comp.d13C.SD.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  71.7 NA NA 5796.9 NA ...
##  $ CatchMassSoil.g.SD  : num  NA NA NA 382 NA ...
##  $ BulkCatch.d13       : num  NA NA NA NA NA ...
##  $ BulkCatch.d13.SD    : num  NA NA NA NA NA ...
##  $ BulkCatch.DD13      : num  NA NA NA NA NA ...
##  $ f.mean.bulk         : num  NA NA NA NA NA ...
##  $ f.mean.bulk.Field   : num  NA NA NA NA NA ...
##  $ f.min.bulk          : num  NA NA NA NA NA ...
##  $ f.min.bulk.Field    : num  NA NA NA NA NA ...
##  $ f.max.bulk          : num  NA NA NA NA NA ...
##  $ f.max.bulk.Field    : num  NA NA NA NA NA ...
##  $ B.mean.bulk         : num  NA NA NA NA NA ...
##  $ B.min.bulk          : num  NA NA NA NA NA ...
##  $ B.max.bulk          : num  NA NA NA NA NA ...
##  $ B.mean.bulk.Field   : num  NA NA NA NA NA ...
##  $ B.min.bulk.Field    : num  NA NA NA NA NA ...
##  $ B.max.bulk.Field    : 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
```

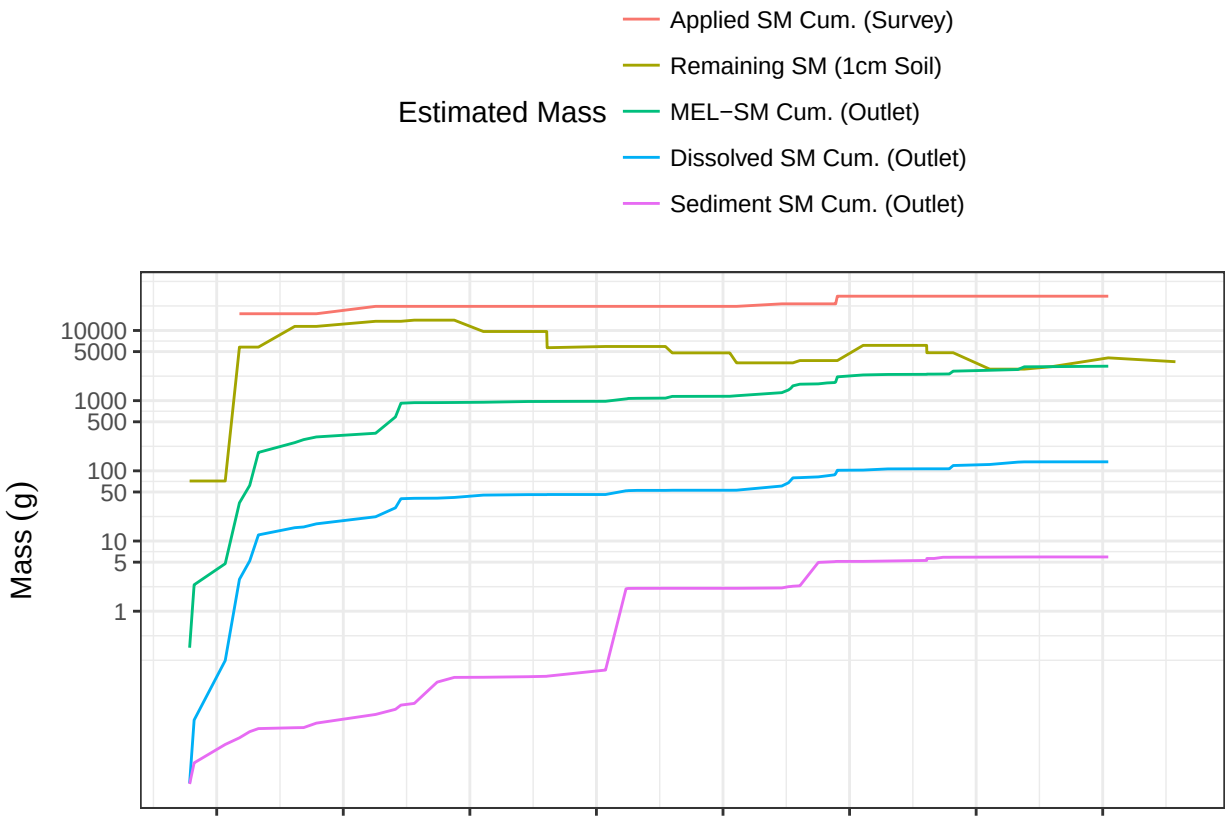
```
# Melt data set
##Subset the necessary columns
soilsRemainMass <- soilsOut[, c("ti" ,"CumAppMass.g", "CumOutDiss.g", "CumOutFilt.g", "CumOutMELsm.g" ,
soilsRemainMass$CumAppMass.g[1:3] <- NA

# 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)", "

pgSimple <- pg[which(pg$variable != ("Dissolved SM Cum. (Outlet)") & pg$variable != ("Sediment SM Cum.
# 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
```

```
## Warning: Removed 7 rows containing missing values (geom_path).
```




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

```
## Warning: Removed 112 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
```

```
## Warning: Removed 5 rows containing missing values (geom_path).
```