

PNAS Figures

PAZ

22 novembre 2016

Required R-packages:

```
# Data wrangling
library("plyr")
library("dplyr")

# Melting data sets & changin axes
library("reshape2")
library("ggrepel")

# Plotting:
library("ggplot2")
library("cowplot")
library("gridExtra")
library("Cairo")
library("GGally")
library("scales")
```

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"
```

Soils

```
weeklySoil = read.csv2("Data/WeeklySoils_Rng.csv", na.strings=c('#DIV/0!', '', 'NA'), header = TRUE)
weeklySoil$Date.ti <- as.POSIXct(strptime(weeklySoil$Date.ti, "%Y-%m-%d %H:%M", tz="EST")) # csv typos,
#weeklySoil$Date.ti <- as.POSIXct(strptime(weeklySoil$Date.ti, "%d/%m/%Y %H:%M", tz="EST"))
sum(is.na(weeklySoil$Date.ti))

## [1] 0

#weeklySoil$Conc.ComSoil.SD <-
# ifelse(weeklySoil$Conc.ComSoil.SD == as.character("#DIV/0!"), NA, as.numeric(as.character(weeklySoil$Conc.ComSoil.SD)))

str(weeklySoil)

## '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.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 ...
```

```
# weeklySoil = weeklySoil %>%
# group_by(Transect) %>%
# arrange(Transect, Wnum)
```

```
weeklySoil$Transect <- factor(weeklySoil$Transect, levels = c("N", "T", "S"))
```

Soil Concentrations

```
#####
```

```
# Concentrations
```

```
#####
```

```
#####
```

```
#####
```

```
#weeklySoil$ti[3] <- as.POSIXct("2016-04-14 08:25:00")
```

```
#weeklySoil$ti[14] <- as.POSIXct("2016-04-14 08:25:00")
```

```
#weeklySoil$ti[24] <- as.POSIXct("2016-04-14 08:25:00")
```

```
#lb1a2 <- paste("App.")
```

```
lbW012 <- paste("App.W0/1/2")
```

```
lbW9 <- paste("App.W9")
```

```
limits_conc_soil <- aes(ymin=Conc.mug.g.dry.soil-Conc.ComSoil.SD, ymax=Conc.mug.g.dry.soil+Conc.ComSoil.SD)
```

```
#limits_conc_soil <- aes(ymin=mean-0.5, ymax=mean+0.5)
```

```
pd <- position_dodge(0.5) # move them .05 to the left and right
```

```
co = ggplot(weeklySoil[1:48, ],
  aes(x=Date.ti, y=Conc.mug.g.dry.soil, colour=Transect, group = Transect)) +
```

```
  geom_point() +
```

```
  geom_line() +
```

```
# Error bars
```

```
  geom_errorbar(limits_conc_soil, width=.1, position=pd) +
```

```

# scale_y_continuous(limits=c(0,10), oob = rescale_none) +

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

scale_x_datetime(breaks = date_breaks("2 weeks"), labels = date_format("%b %d")) +
ylab(expression(paste("Conc. S-Meto. ", {({\mu}*g / g.soil.dry)}))) +
# facet_wrap(~Transect, nrow = 3) +
# xlab("Date") +
# theme(axis.text.x=element_text(angle = 45, hjust = 1)) +
# scale_x_datetime(breaks = date_breaks("2 weeks"), labels = date_format("%b %d")) +

# Smooth linear models
# stat_smooth(method = "lm", formula = y ~ poly(x, 2)) +
# stat_smooth(method = "lm") +

# Text
# W0 Application
# annotate("text", x = as.POSIXct('2016-03-25 08:04:00'), y = 4, label = lb1a2, parse = T, size = 3.0)
geom_segment(aes(x = as.POSIXct('2016-04-14 08:04:00'), y = 0.5, xend = as.POSIXct('2016-03-26 01:04:00'),
                 arrow = arrow(length = unit(0.2, "cm")))) +

# W1 Application
geom_segment(aes(x = as.POSIXct('2016-04-14 08:04:00'), y = 0.5,
                 xend = as.POSIXct('2016-04-05 08:04:00'), yend = 0), color = "black",
             arrow = arrow(length = unit(0.2, "cm")))) +

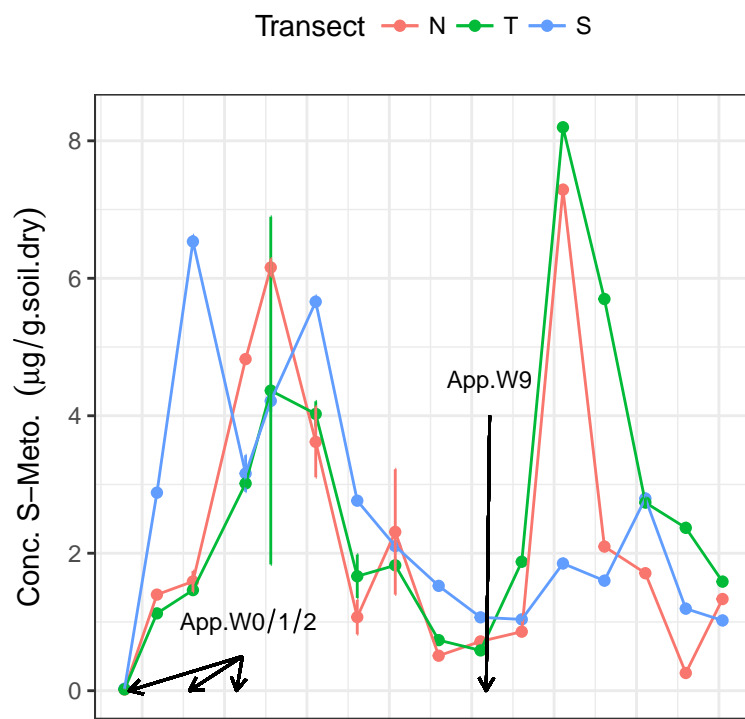
# W2 Application
annotate("text", x = as.POSIXct('2016-04-15 08:04:00'), y = 1, label = lbW012, parse = T, size = 3.0)
geom_segment(aes(x = as.POSIXct('2016-04-14 08:04:00'), y = 0.5,
                 xend = as.POSIXct('2016-04-13 08:04:00'), yend = 0), color = "black",
             arrow = arrow(length = unit(0.2, "cm")))) +

# W9 Application
annotate("text", x = as.POSIXct('2016-05-26 08:04:00'), y = 4.5, label = lbW9, parse = T, size = 3.0)
geom_segment(aes(x = as.POSIXct('2016-05-26 08:04:00'), y = 4,
                 xend = as.POSIXct('2016-05-25 18:04:00'), yend = 0), color = "black",
             arrow = arrow(length = unit(0.2, "cm"))))

#geom_text_repel(aes(label=Wnum),
#               # size = 3,
#               # arrow = arrow(length = unit(0.005, 'npc'), type = "closed"),
#               # force = 0.5,
#               # point.padding = unit(0.5, 'lines'),
#               # max.iter = 2e3,
#               # nudge_x = .05)

```

co



```
# Linear model
# ggsave(co, filename = "CompositeConcLM.png", width = 7, height = 5, units = "in", scale = 1)

ggsave(co, filename = "CompositeConcLM.tiff", height = 10, width = 8.7, units = 'cm')

# No linear model
# ggsave(co, filename = "CompositeConc.png", width = 7, height = 5, units = "in", scale = 1)
```

Soil isotope signatures

```
initialDelta = -31.21
weeklySoil$DD13C.comp <- (weeklySoil$comp.d13C - (initialDelta))

limits_dCsoil <- aes(ymin=comp.d13C-comp.d13C.SD, ymax=comp.d13C+comp.d13C.SD)
#limits_dCsoil <- aes(ymin=comp.d13C-0.5, ymax=comp.d13C+0.5)
lb1a <- paste("App.-S-meto.")
lb1ab <- paste("delta^{13}~C:-31.21")
lb1a2 <- paste("App. ")

lbW012 <- paste("App.W0/1/2")
lbW9 <- paste("App.W9")

isCo = ggplot(weeklySoil, aes(x=Date.ti, y=comp.d13C, colour=Transect, group = Transect)) +
  geom_errorbar(limits_dCsoil, width=.05) +
  geom_point() +
  theme_bw() +
  #stat_smooth(method = "lm", formula = y ~ poly(x, 2)) +
```

```

stat_smooth(method = "lm") +
facet_wrap(~Transect, nrow = 3) +
xlab("Date") +
theme(axis.text.x=element_text(angle = 45, hjust = 1)) +
#ylab(expression(paste({delta}^"13", "C", ' \u2113'))) +
ylab(expression(paste({delta}^"13", "C", ' (\u2030)'))) +
scale_y_continuous(breaks=seq(-34,-21,2)) +
geom_hline(yintercept = -31.21, color = "dodgerblue4", linetype = "dotted") +
geom_hline(yintercept = -30.71, color = "dodgerblue3", linetype = "dotted") +
geom_hline(yintercept = -31.71, color = "dodgerblue3", linetype = "dotted") +
annotate("text", x = as.POSIXct('2016-04-05 22:04:00'), y = -22.5, label = lb1a, parse = T, size = 3.0)
annotate("text", x = as.POSIXct('2016-04-05 22:04:00'), y = -23.5, label = lb1ab, parse = T, size = 3.0)

annotate("text", x = as.POSIXct('2016-03-25 08:04:00'), y = -29, label = lb1a2, parse = T, size = 3.0)
geom_segment(aes(x = as.POSIXct('2016-03-25 08:04:00'), y = -29.8,
                    xend = as.POSIXct('2016-03-25 08:04:00'), yend = -31.0),
              arrow = arrow(length = unit(0.2, "cm")) +
              annotate("text", x = as.POSIXct('2016-04-03 00:04:00'), y = -29, label = lb1a2, parse = T, size = 3.0)
geom_segment(aes(x = as.POSIXct('2016-04-03 00:04:00'), y = -29.8,
                    xend = as.POSIXct('2016-04-05 08:04:00'), yend = -31.0),
              arrow = arrow(length = unit(0.2, "cm")) +
              annotate("text", x = as.POSIXct('2016-04-13 08:04:00'), y = -25, label = lb1a2, parse = T, size = 3.0)
geom_segment(aes(x = as.POSIXct('2016-04-13 08:04:00'), y = -26,
                    xend = as.POSIXct('2016-04-13 08:04:00'), yend = -31.0),
              arrow = arrow(length = unit(0.2, "cm")) +
              annotate("text", x = as.POSIXct('2016-05-26 08:04:00'), y = -29, label = lb1a2, parse = T, size = 3.0)
geom_segment(aes(x = as.POSIXct('2016-05-26 08:04:00'), y = -29.8,
                    xend = as.POSIXct('2016-05-25 08:04:00'), yend = -31.0),
              arrow = arrow(length = unit(0.2, "cm")) +
              #scale_x_continuous(breaks=seq(0,11,1)) +
              scale_x_datetime(breaks = date_breaks("2 weeks"), labels = date_format("%b %d")) +

              #annotate("text", x = as.POSIXct('2016-05-30 20:04:00'), y = -30.5, label = lb1a, parse = T, size = 2)
              theme(legend.position = "top")

# isCo

# Linear model (LM)
# ggsave(isCo, filename = "CompositeIsotopesLM.png", width = 7, height = 5, units = "in", scale = 1)
# No linear model
# ggsave(isCo, filename = "CompositeIsotopes.png", width = 7, height = 5, units = "in", scale = 1)

# View(weeklySoil)

# Ommitted, graph is tautological.
### Delta vs. f (Soils)
soilf = ggplot(weeklySoil, aes(x=f.comp, y=DD13C.comp, colour=Transect, group = Transect)) +
  #geom_errorbar(limits_dCsoil, width=.05) +
  geom_point() +
  theme_bw() +
  stat_smooth(method = "lm", formula = y ~ poly(x, 2)) +
  #stat_smooth(method = "lm") +

```

```

facet_wrap(~Transect, nrow = 3) +
scale_x_reverse() +
xlab("Fraction remaining (f)") +
theme(axis.text.x=element_text(angle = 45, hjust = 1)) +
#ylab(expression(paste({delta}^"13", "C", ' \211')))) +
ylab(expression(paste({Delta~delta}^"13", "C", ' (\u2030)')))) +
#scale_y_continuous(breaks=seq(-34,-21,2)) +
theme(legend.position = "top") +
#geom_text_repel(aes(label=WeekNo, color = factor(Transect)),
#               #arrow = arrow(length = unit(0.005, 'npc'), type = "closed"),
#               #force = 1,
#               #point.padding = unit(1.0, 'lines'),
#               #max.iter = 2e3,
#               #nudge_x = .2) +

geom_point()

# soilf

#####
#####
#####
### DeltaDelta vs time
#####
# View(weeklySoil)
# limits_DdCsoil <- aes(ymin=comp.d13C-comp.d13C.SD-initialDelta, ymax=comp.d13C+comp.d13C.SD-initialDelta)
limits_DdCsoil <- aes(ymin=comp.d13C-comp.d13C.SE-initialDelta, ymax=comp.d13C+comp.d13C.SE-initialDelta)
# pd <- position_dodge(0.5)
# A0df[1:27,]
deltaTime = ggplot(weeklySoil[1:48, ], aes(x=Date.ti, y=DD13C.comp, colour=Transect, group = Transect)) +
  geom_errorbar(limits_DdCsoil, width=.5) +
  geom_point() +

# Themes and axes
theme_bw() +
theme(legend.position="none",
      # axis.title.x = element_blank(),
      axis.text.x=element_text(angle = 45, hjust = 1)
    ) +
xlab("Date") +
scale_x_datetime(breaks = date_breaks("2 weeks"), labels = date_format("%b %d")) +

ylab(expression(paste({Delta~delta}^"13", "C", ' (\u2030)')))) +
scale_y_continuous(breaks=seq(0, 8, 1)) +
# ylab(expression(paste({delta}^"13", "C", ' \211')))) +
# ylab(expression(paste({delta}^"13", "C", ' (\u2030)')))) +
# facet_wrap(~Transect, nrow = 3) +

# Smooth linear models
stat_smooth(method = "lm", se=FALSE) +
# stat_smooth(method = "lm", formula = y ~ poly(x, 2)) +
# stat_smooth(data=subset(weeklySoil[4:27, ]), method = "lm", formula = y~x, se=F) +
# stat_smooth(data=subset(weeklySoil[18:36, ]), method = "lm", formula = y~x, se=F) +

```

```

# Text
# Application W0
annotate("text",
  x = as.POSIXct('2016-04-04 01:04:00'), y = 6, label = lbW012, parse = T, size = 3.0) +
geom_segment(aes(x = as.POSIXct('2016-04-03 08:04:00'), y = 5.5,
  xend = as.POSIXct('2016-03-25 22:04:00'), yend = -0), color = "black",
  arrow = arrow(length = unit(0.2, "cm")))) +
#annotate("text",
#  x = as.POSIXct('2016-04-03 00:04:00'), y = 2, label = lb1a2, parse = T, size = 3.0) +

# Application W1
geom_segment(aes(x = as.POSIXct('2016-04-03 08:04:00'), y = 5.5,
  xend = as.POSIXct('2016-04-05 08:04:00'), yend = 0), color = "black",
  arrow = arrow(length = unit(0.2, "cm")))) +
# annotate("text", x = as.POSIXct('2016-04-15 08:04:00'), y = 1, label = lb1a2, parse = T, size = 3.0) +

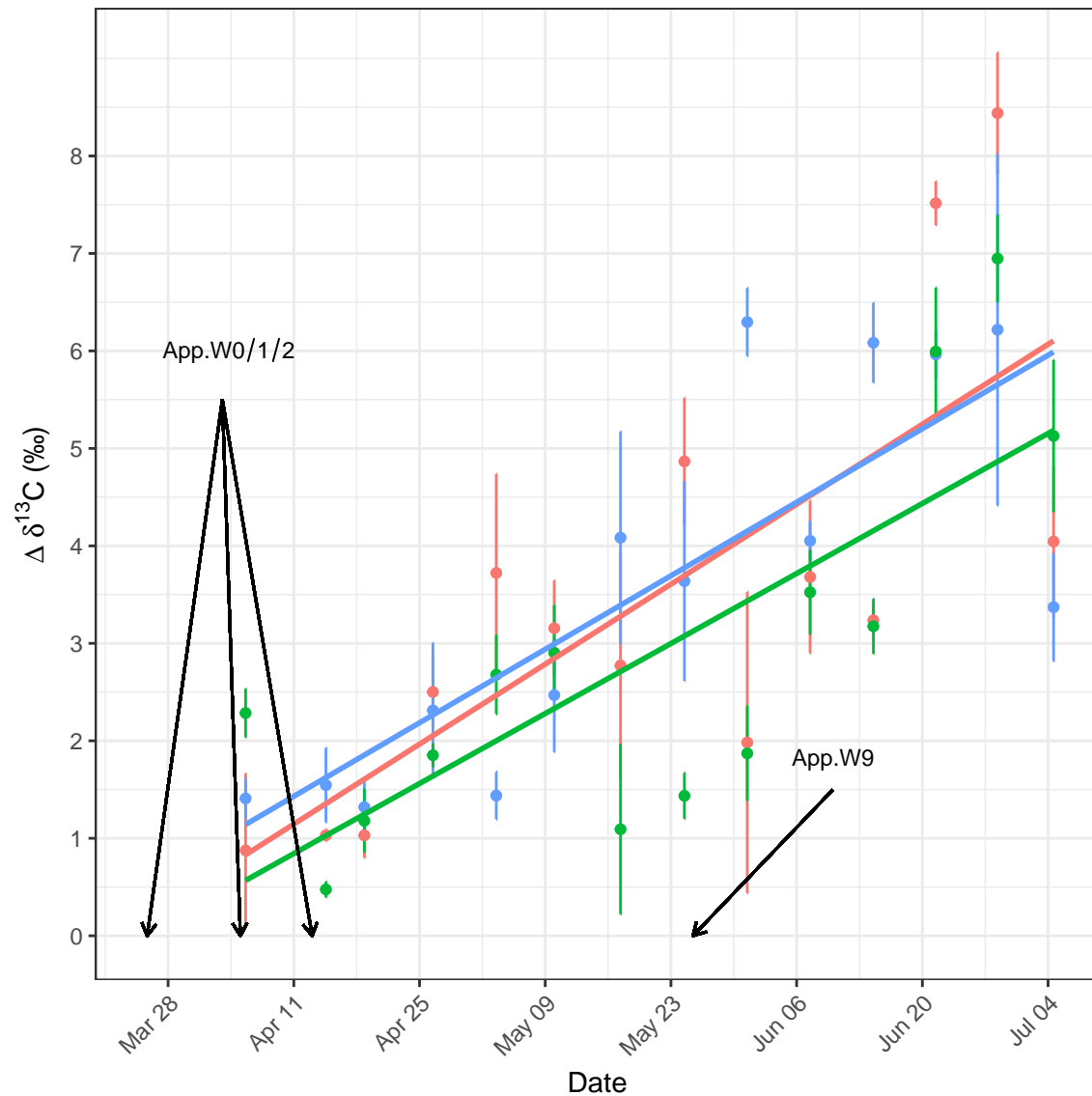
# Application W2
geom_segment(aes(x = as.POSIXct('2016-04-03 08:04:00'), y = 5.5,
  xend = as.POSIXct('2016-04-13 08:04:00'), yend = 0), color = "black",
  arrow = arrow(length = unit(0.2, "cm")))) +

# Application W9
annotate("text",
  x = as.POSIXct('2016-06-10 08:04:00'), y = 1.8, label = lbW9, parse = T, size = 3.0) +
geom_segment(aes(x = as.POSIXct('2016-06-10 08:04:00'), y = 1.5,
  xend = as.POSIXct('2016-05-25 18:04:00'), yend = 0), color = "black",
  arrow = arrow(length = unit(0.2, "cm")))) # +

#geom_text_repel(aes(label=Wnum, color = factor(Transect)),
#  #
#    arrow = arrow(length = unit(0.005, 'npc'), type = "closed"),
#  #
#    force = 1,
#  #
#    point.padding = unit(1.0, 'lines'),
#  #
#    max.iter = 2e3,
#  #
#    nudge_x = .2)

deltaTime

```



```
#soils = plot_grid(co, deltaTime, ncol = 1, nrow = 2, align = "v")
#soils
```

Degradation

```
lb1a2 <- paste("App.")

lb1b <- paste("(A)~epsilon:-1.5")
lb1b2 <- paste("(B)~epsilon:-2.0")

Bsoil =ggplot(weeklySoil)+
  #geom_errorbar(limits_dCsoil, width=.05) +
  #geom_point(aes(x=Date.ti, y=B.comp, colour=Transect, group = Transect)) +
  geom_point(aes(x=Date.ti, y=B.min.comp, colour=Transect, group = Transect)) + #, color = "dodgerblue4"
```



```

theme_bw() +
# stat_smooth(method = "lm", formula = y ~ poly(x, 2)) +
#stat_smooth(aes(x=Date.ti, y=B.min.comp), method = "lm", se = F, color = "dodgerblue4") +
#stat_smooth(aes(x=Date.ti, y=B.comp), method = "lm", se = F, color = "grey40") +

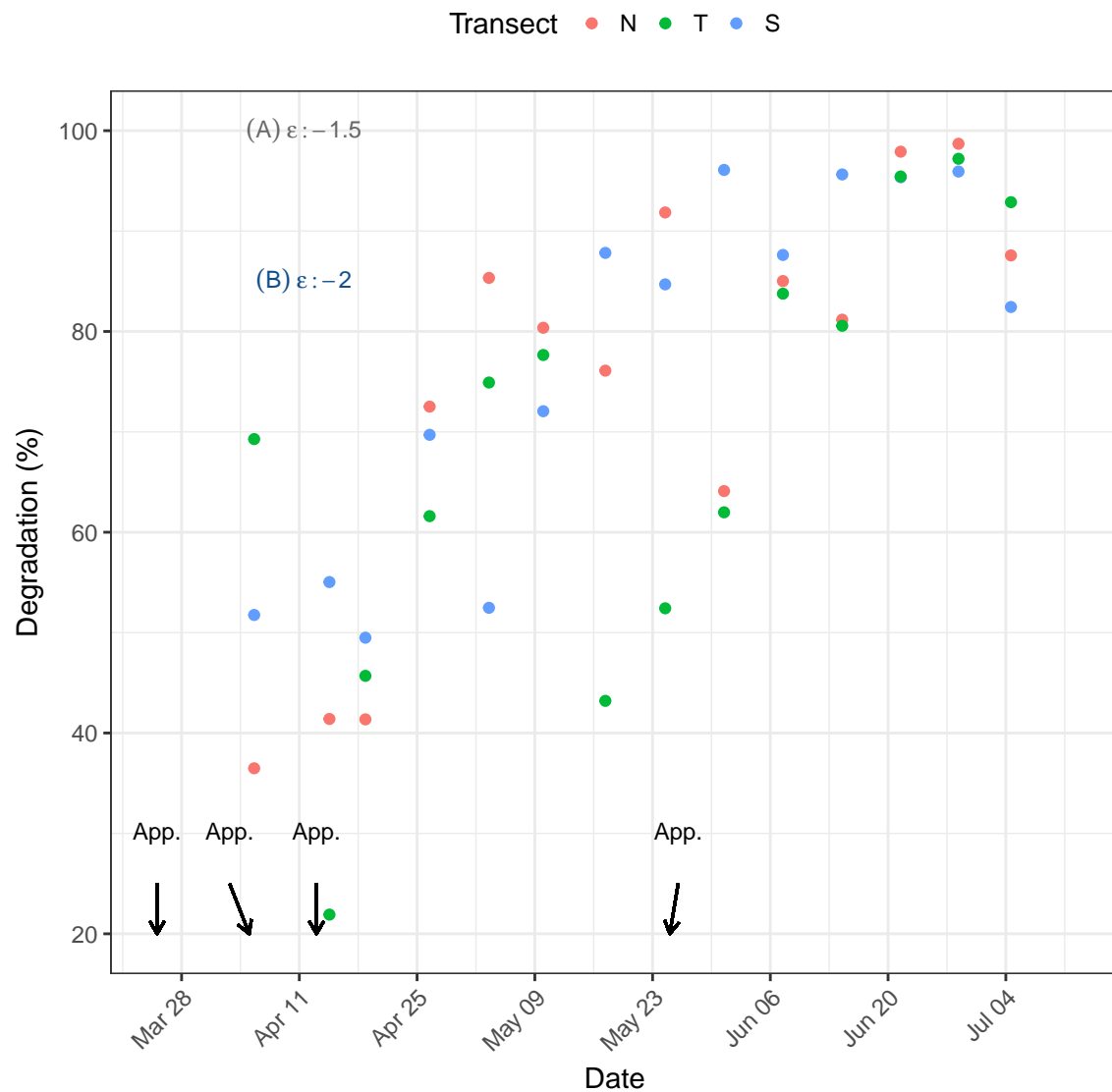
# Individual / broken lines
#geom_smooth(data=subset(weeklySoil[10:27, ]), aes(x=Date.ti, y=B.min.comp), method = "lm", se = F, c
#geom_smooth(data=subset(weeklySoil[31:45, ]), aes(x=Date.ti, y=B.min.comp), method = "lm", se = F, c
#geom_smooth(data=subset(weeklySoil[10:27, ]), aes(x=Date.ti, y=B.comp), method = "lm", se = F, color
#geom_smooth(data=subset(weeklySoil[31:45, ]), aes(x=Date.ti, y=B.comp), method = "lm", se = F, color

# Continous lines
# geom_smooth(data=subset(weeklySoil[1:45, ]), aes(x=Date.ti, y=B.min.comp), method = "lm", formula =
# geom_smooth(y=B.min.comp, method = "lm", formula = y ~ poly(x, 2)) +
# facet_wrap(~Transect, nrow = 3) +
xlab("Date") +
theme(axis.text.x=element_text(angle = 45, hjust = 1)) +
#ylab(expression(paste({delta}~"13", "C", ' \211')))) +
ylab("Degradation (%)") +
scale_y_continuous(breaks=seq(0, 100, 20)) +
#geom_hline(yintercept = -31.47, color = "dodgerblue4", linetype = "dotted") +
#geom_hline(yintercept = -30.97, color = "dodgerblue3", linetype = "dotted") +
#geom_hline(yintercept = -31.97, color = "dodgerblue3", linetype = "dotted") +
annotate("text", x = as.POSIXct('2016-04-11 20:04:00'), y = 100, label = lb1b, parse = T, size = 3.0,
annotate("text", x = as.POSIXct('2016-04-11 20:04:00'), y = 85, label = lb1b2, parse = T, size = 3.0,

annotate("text", x = as.POSIXct('2016-03-25 08:04:00'), y = 30, label = lb1a2, parse = T, size = 3.0)
geom_segment(aes(x = as.POSIXct('2016-03-25 08:04:00'), y = 25,
xend = as.POSIXct('2016-03-25 08:04:00'), yend = 20),
arrow = arrow(length = unit(0.2, "cm")))) +
annotate("text", x = as.POSIXct('2016-04-03 00:04:00'), y = 30, label = lb1a2, parse = T, size = 3.0)
geom_segment(aes(x = as.POSIXct('2016-04-03 00:04:00'), y = 25,
xend = as.POSIXct('2016-04-05 08:04:00'), yend = 20),
arrow = arrow(length = unit(0.2, "cm")))) +
annotate("text", x = as.POSIXct('2016-04-13 08:04:00'), y = 30, label = lb1a2, parse = T, size = 3.0)
geom_segment(aes(x = as.POSIXct('2016-04-13 08:04:00'), y = 25,
xend = as.POSIXct('2016-04-13 08:04:00'), yend = 20),
arrow = arrow(length = unit(0.2, "cm")))) +
annotate("text", x = as.POSIXct('2016-05-26 08:04:00'), y = 30, label = lb1a2, parse = T, size = 3.0)
geom_segment(aes(x = as.POSIXct('2016-05-26 08:04:00'), y = 25,
xend = as.POSIXct('2016-05-25 08:04:00'), yend = 20),
arrow = arrow(length = unit(0.2, "cm")))) +
scale_x_datetime(breaks = date_breaks("2 weeks"), labels = date_format("%b %d")) +
#scale_x_continuous(breaks=seq(0,11,1)) +
theme(legend.position = "top")

```

Bsoil



```
# Linear model
ggsave(Bsoil, filename = "CompositeDegradationLM.png", width = 7, height = 5, units = "in", scale = 1)

#deltaCo = plot_grid(co, isCo, ncol = 2, nrow = 1, align = "h")
# deltaCoBio = plot_grid(co, isCo, Bsoil, ncol = 3, nrow = 1, align = "h")
# deltaCoBio

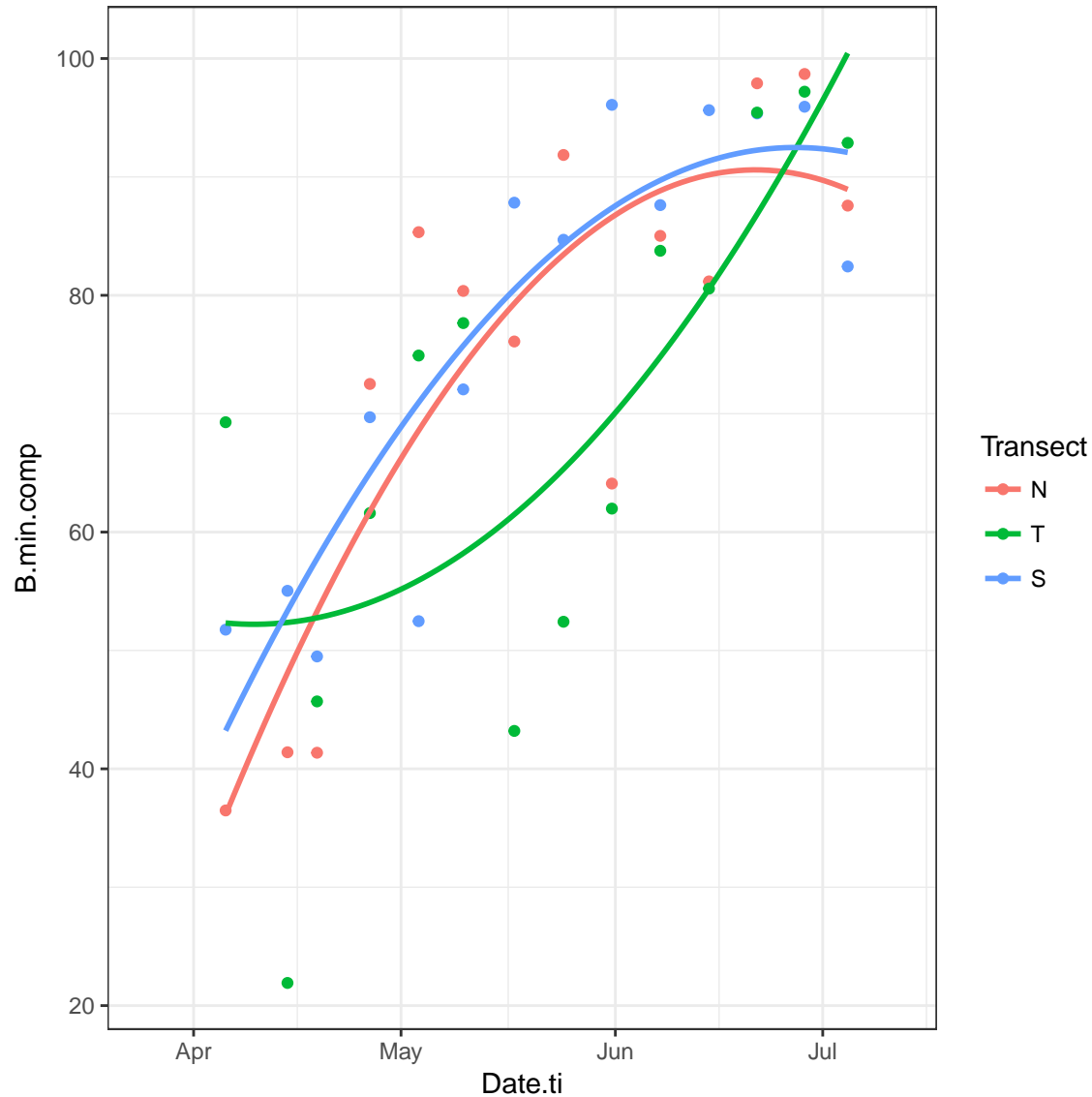
# Linear model
#ggsave(deltaCo, filename = "CompositeConcLM.png", width = 6, height = 7, units = "in", scale = 1)
#ggsave(deltaCoBio, filename = "SoilConcDeltBio_LM.png", width = 11.69, height = 8.27, units = "in", scale = 1)

# No linear model
#ggsave(deltaCo, filename = "CompositeConc.png", width = 6, height = 7, units = "in", scale = 1)

# weeklySoil2 = weeklySoil[1:45, ]
# View(weeklySoil2)
```

```
Bsoil2 = ggplot(weeklySoil, aes(x=Date.ti, y=B.min.comp, colour=Transect, group = Transect)) +
  geom_point() +
  # geom_point(aes(x=Date.ti, y=B.comp, colour=Transect, group = Transect)) +
  theme_bw() +
  stat_smooth(method = "lm", formula = y ~ poly(x, 2), se=FALSE)
```

Bsoil2



Water

```
A0df = read.csv2("Data/WeeklyHydroContam_R.csv")
str(A0df)
```

```
## 'data.frame':   51 obs. of  69 variables:
## $ ti           : Factor w/ 51 levels "2016-03-25 00:04:00",...: 1 2 3 4 5 6 7 8 9 10 ...
```

```

## $ WeekSubWeek      : Factor w/ 51 levels "W0-0x","W0-1",...: 1 2 3 4 5 6 26 27 28 29 ...
## $ tf               : Factor w/ 51 levels "2016-03-25 12:02:00",...: 1 2 3 4 5 6 7 8 9 10 ...
## $ iflux            : num  1.25 1.12 1.31 1.46 16.33 ...
## $ fflux            : num  1.13 1.31 1.46 16.45 15.18 ...
## $ changeflux       : num  -0.119 0.189 0.148 14.989 -1.15 ...
## $ maxQ              : num  1.25 1.38 1.64 38.4 18.67 ...
## $ minQ              : num  1.118 1.082 0.929 1.449 13.201 ...
## $ Duration.Hrs      : num  12 82.5 37.6 27.3 23.1 ...
## $ chExtreme         : num  -0.13 0.256 0.33 36.944 -3.133 ...
## $ AveDischarge.m3.h : num  1.2 1.21 1.28 14.32 15.53 ...
## $ Volume.m3         : num  14.4 100.2 48.3 390.4 359.2 ...
## $ Sampled.Hrs       : num  12 82.5 37.6 27.3 23.1 ...
## $ Sampled           : Factor w/ 2 levels "Not Sampled",...: 1 2 1 2 2 1 2 2 1 2 ...
## $ Conc.mug.L        : num  0.246 0.246 3.517 6.788 6.561 ...
## $ Conc.SD           : num  NA 0.0193 NA 0.2894 0.1906 ...
## $ OXA_mean          : num  4.82 4.82 17.68 30.53 32.49 ...
## $ OXA_SD            : num  NA 1.141 NA 10.185 0.243 ...
## $ ESA_mean          : num  18.1 18.1 32 46 41.3 ...
## $ ESA_SD            : num  NA 3.497 NA 3.037 0.853 ...
## $ N.x               : int  NA 3 NA 3 3 NA 3 3 NA 3 ...
## $ diss.d13C         : num  NA -26.7 NA -30.5 -30.6 ...
## $ SD.d13C           : num  NA 0.936 NA 0.106 0.151 ...
## $ se.d13C           : num  NA 0.5403 NA 0.0612 0.0874 ...
## $ MES.mg.L          : num  NA 53.4 NA 62.5 22.5 ...
## $ MES.sd            : num  NA NA NA NA NA NA NA NA NA NA ...
## $ MO.mg.L           : num  NA 0 NA 0.001 0.0001 NA 0.0001 0.0001 NA 0.0058 ...
## $ Conc.Solids.mug.gMES: num  0.645 0.645 0.385 0.126 0.436 ...
## $ N.y               : int  NA NA NA NA NA NA NA 3 3 NA NA ...
## $ filt.d13C         : num  NA NA NA NA NA ...
## $ filt.SD.d13C      : num  NA NA NA NA NA ...
## $ filt.se.d13C      : num  NA NA NA NA NA ...
## $ DD13C.diss        : num  NA 4.545 NA 0.741 0.59 ...
## $ DD13C.filt        : num  NA NA NA NA NA ...
## $ f.diss            : num  NA 0.0689 NA 0.6459 0.706 ...
## $ f.filt            : num  NA NA NA NA NA ...
## $ B.diss            : num  NA 93.1 NA 35.4 29.4 ...
## $ B.filt            : num  NA NA NA NA NA ...
## $ NH4.mM            : num  NA NA NA 0.05 NA NA NA NA NA NA ...
## $ TIC.ppm.filt      : num  NA NA NA 51.8 44.8 NA 66.7 52.1 NA 69.4 ...
## $ Cl.mM             : num  NA NA NA 1.48 1574 ...
## $ NO3...mM          : num  NA NA NA 616 778 ...
## $ PO4..mM           : int  NA NA NA NA NA NA NA NA NA NA ...
## $ NPOC.ppm          : num  NA NA NA 4 4.4 NA 5.8 3.4 NA 9.1 ...
## $ TIC.ppm.unfilt    : num  NA NA NA 44.8 26.4 NA 39 32.3 NA 54.8 ...
## $ TOC.ppm.unfilt    : num  NA NA NA 4.7 5.4 NA 2.7 3.8 NA 3.9 ...
## $ ExpMES.Kg         : num  5.35 5.35 14.88 24.4 8.08 ...
## $ DissSmeto.mg      : num  3.54 24.6 170.04 2649.91 2357 ...
## $ DissOXA.mg        : num  69.5 483.2 854.7 11918.4 11672.7 ...
## $ DissESA.mg        : num  260 1808 1548 17951 14830 ...
## $ FiltSmeto.mg      : num  3.45 3.45 5.73 3.07 3.52 ...
## $ TotMassOut.mg     : num  6.99 28.06 175.77 2652.98 2360.52 ...
## $ FracDiss          : num  0.506 0.877 0.967 0.999 0.999 ...
## $ FracFilt          : num  0.49352 0.12301 0.03261 0.00116 0.00149 ...
## $ Appl.Mass.g       : num  6369 0 0 0 0 ...

```

```
## $ CumAppMass.g : num 6369 6369 6369 6369 6369 ...
## $ SimOutDiss.g : num 0.00354 0.0246 0.17004 2.64991 2.357 ...
## $ SimOutFilt.g : num 0.00345 0.00345 0.00573 0.00307 0.00352 ...
## $ SimOutOXA.g : num 0.0695 0.4832 0.8547 11.9184 11.6727 ...
## $ SimOutESA.g : num 0.26 1.81 1.55 17.95 14.83 ...
## $ SimOutSmeto.g : num 0.00699 0.02806 0.17577 2.65298 2.36052 ...
## $ SimMELsm.g : num 0.302 2.078 2.379 30.241 27.008 ...
## $ 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 ...
## $ CumOutSmeto.g : num 0.00699 0.03505 0.21082 2.8638 5.22432 ...
## $ CumOutMELsm.g : num 0.302 2.38 4.76 35.001 62.009 ...
## $ BalMassDisch.g : num 6369 6367 6365 6334 6307 ...
## $ prctMassOut : num 4.98e-05 2.00e-04 1.25e-03 1.89e-02 1.68e-02 ...
## $ FracDeltaOut : num 0 -0.00533 0 -0.57576 -0.51483 ...
```

```
# Adding a Weeks column for labelling
```

```
A0df$WeekSubWeek <- as.character(A0df$WeekSubWeek)
```

```
Split <- strsplit(A0df$WeekSubWeek, "-", fixed = TRUE)
```

```
A0df$Weeks <- sapply(Split, "[", 1)
```

```
A0df$WeekSubWeek <- factor(A0df$WeekSubWeek, levels = unique(A0df$WeekSubWeek))
```

```
A0df$Weeks <- factor(A0df$Weeks, levels = unique(A0df$Weeks))
```

```
A0df$ti <- as.POSIXct(strptime(A0df$ti, "%Y-%m-%d %H:%M", tz="EST"))
```

```
sum(is.na(A0df$ti))
```

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

Outlet - Concentrations

```
# View(A0df)
```

```
limits_conc <- aes(ymin=Conc.mug.L-Conc.SD, ymax=Conc.mug.L+Conc.SD, color = Weeks, group = Weeks)
```

```
conc1 <- ggplot(A0df, aes(x=ti, y=Conc.mug.L)) +
  geom_point( aes(color = Weeks, group = Weeks)) +
```

```
# Error bars
```

```
geom_errorbar(limits_conc, width=1) +
```

```
# 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"
    )+
```

```
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("Conc. S-Meto. ", {({mu}*g / L)}))) +
```

```
scale_y_continuous(breaks = c(18,16,14,12,10, 8, 6, 4, 2, 0), limits = c(-1, 18) ) +
```

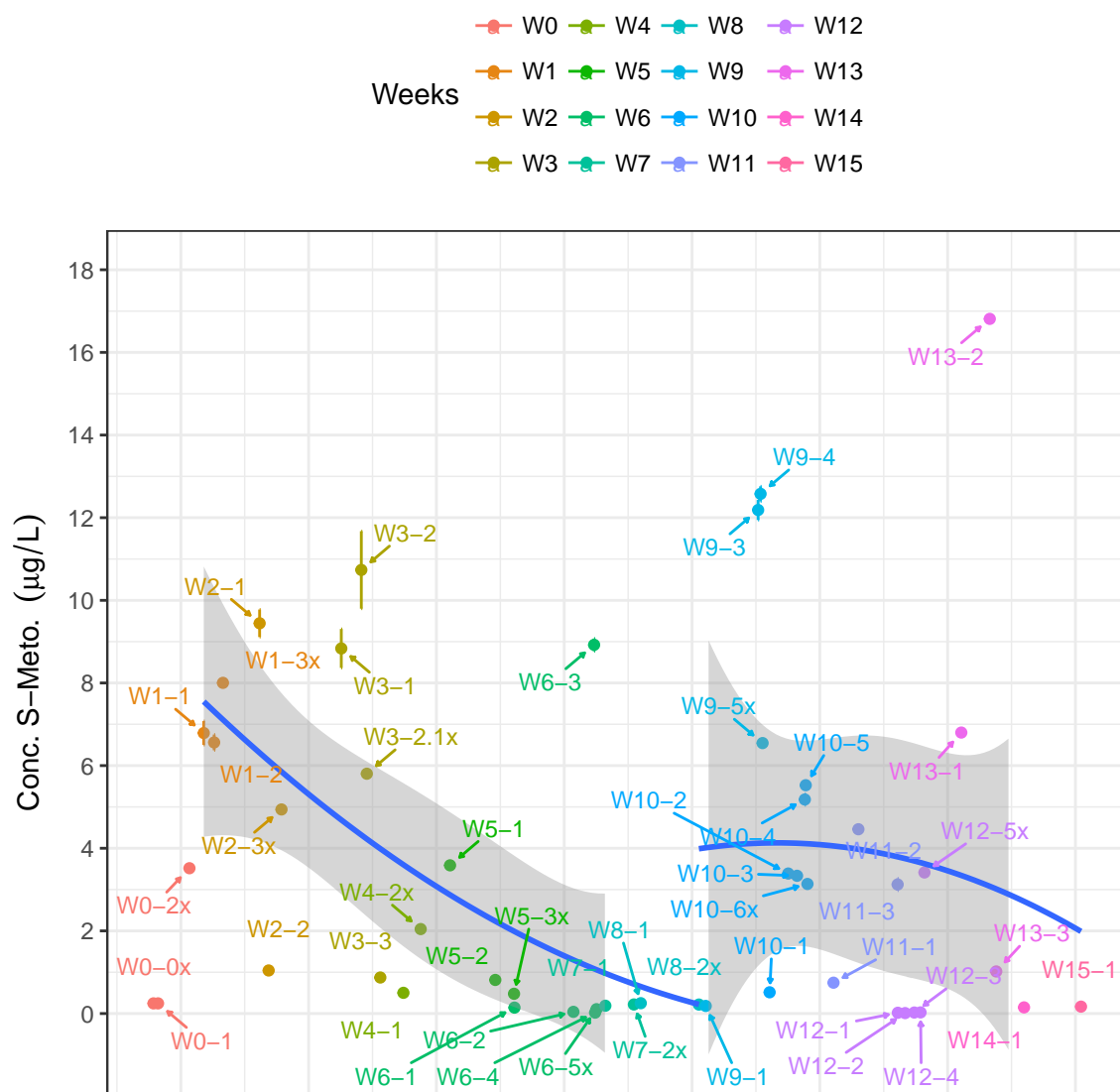
```

# Smooth linear models
geom_smooth(data=subset(AOdf[4:27, ]), method = "lm", formula = y ~ poly(x, 2)) +
geom_smooth(data=subset(AOdf[27:length(AOdf), ]), method = "lm", formula = y ~ poly(x, 2)) +

# Text
# Application W9
# annotate("text",
#         x = as.POSIXct('2016-06-10 08:04:00'), y = -1, label = lbw9, parse = T, size = 3.0) +
# geom_segment(aes(x = as.POSIXct('2016-06-05 08:04:00'), y = -1,
#                 xend = as.POSIXct('2016-05-25 18:04:00'), yend = -0.9), color = "black",
#             arrow = arrow(length = unit(0.2, "cm")))) +
geom_text_repel(aes(label=WeekSubWeek, color = factor(Weeks)), # WeekSubWeek or Weeks
               size = 3,
               arrow = arrow(length = unit(0.005, 'npc'), type = "closed"),
               force = 0.5,
               point.padding = unit(0.5, 'lines'),
               max.iter = 2e3,
               nudge_x = .05)

```

conc1



```

conc2 <- ggplot(AOdf[28:length(AOdf),], aes(x=ti, y=Conc.mug.L)) +
  geom_point( aes(color = Weeks, group = Weeks)) +
  # Error bars
  # geom_errorbar(aes(ymin=mean.d13C-SD.d13C, ymax=mean.d13C+SD.d13C), width=.1) +
  geom_errorbar(limits_conc, width=1) +

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

```

```

    plot.margin = unit(c(0,3.5,0,0), "lines")) +
#scale_x_datetime(breaks = date_breaks("week"), labels = date_format("%m/%d")) +
scale_y_continuous(breaks = c(20,15,10,5,0), limits = c(-5, 20) ) +
xlab("Date") +
ylab("") +

# Smooth linear models
stat_smooth(method = "lm", formula = y ~ poly(x, 2)) +
#geom_hline(yintercept = -31.21, color = "dodgerblue4", linetype = "dotted") +
#geom_hline(yintercept = -30.71, color = "dodgerblue3", linetype = "dotted") +
#geom_hline(yintercept = -31.71, color = "dodgerblue3", linetype = "dotted") +

# Text
#annotate("text", x = as.POSIXct('2016-06-25 00:04:00'), y = -31.2, label = lb1, parse = T) +
annotate("text", x = as.POSIXct('2016-05-27 08:04:00'), y = -3, label = "App.4", parse = T) +
geom_segment(aes(x = as.POSIXct('2016-05-26 08:04:00'), y = -4,
                  xend = as.POSIXct('2016-05-26 08:04:00'), yend = -5.0),
              arrow = arrow(length = unit(0.2, "cm")))) +
geom_text_repel(aes(label=Weeks, color = factor(Weeks)),
                size = 3,
                arrow = arrow(length = unit(0.005, 'npc'), type = "closed"),
                force = 0.5,
                point.padding = unit(0.5, 'lines'),
                max.iter = 2e3,
                nudge_x = .05)

#concs = plot_grid(conc1, conc2, ncol = 2, nrow = 1, align = "h")
#concs

```

Outlet Isotopes - Continous

```

A0df$SD.d13C.err <- ifelse(is.na(A0df$SD.d13C), 0.5, A0df$SD.d13C)
# limits_dC <- aes(ymin=diss.d13C-SD.d13C.err, ymax=diss.d13C+SD.d13C.err, color = Weeks, group = Weeks)
limits_dC <- aes(ymin=diss.d13C-SD.d13C, ymax=diss.d13C+SD.d13C, color = Weeks, group = Weeks)
# View(A0df)

iso <- ggplot(A0df, aes(x=ti, y=diss.d13C)) +
  #geom_errorbar(aes(ymin=mean.d13C-SD.d13C, ymax=mean.d13C+SD.d13C), width=.1) +
  geom_errorbar(limits_dC, width=1) +
  #theme_gray() +
  theme_bw() +
  theme(axis.text.x=element_text(angle = 45, hjust = 1)) +
#scale_x_datetime(breaks = date_breaks("week"), labels = date_format("%m/%d")) +
  geom_point( aes(color = Weeks, group = Weeks)) +
  #stat_smooth(method = "lm", formula = y ~ x) +
  geom_smooth(data=subset(A0df[4:length(A0df), ]), method = "lm", formula = y ~ poly(x, 2)) +
  #stat_smooth(method = "lm", formula = y ~ poly(x, 2)) +
  #theme(axis.text.x = element_blank()) +
  #theme(plot.margin = unit(c(1,1,1,1), "lines")) +
  geom_hline(yintercept = -31.21, color = "dodgerblue4", linetype = "dotted") +
  geom_hline(yintercept = -30.71, color = "dodgerblue3", linetype = "dotted") +

```

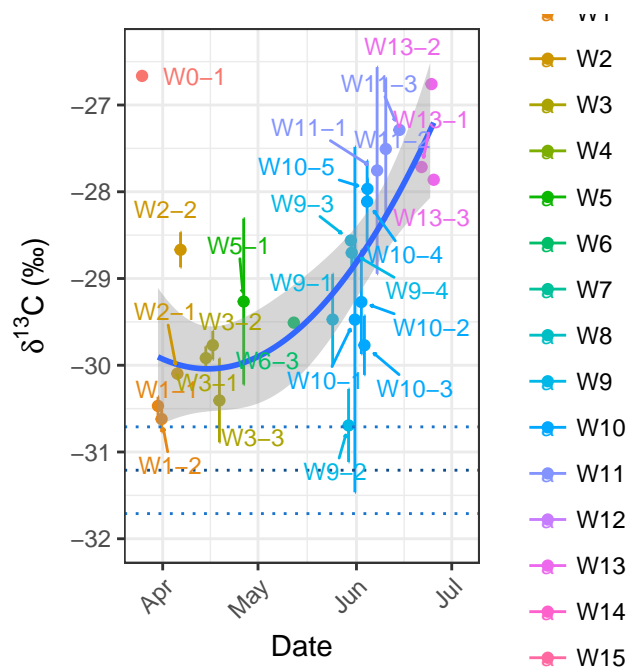


```

geom_hline(yintercept = -31.71, color = "dodgerblue3", linetype = "dotted") +
#annotate("text", x = as.POSIXct('2016-06-25 00:04:00'), y = -31.2, label = lb1, parse = T) +
xlab("Date") +
#theme(legend.position="top") +
scale_y_continuous(breaks = c(-32,-31,-30,-29, -28, -27), limits = c(-32, -26.4) ) +
ylab(expression(paste({delta}^13,"C", ' (\u2030)'))) +
geom_text_repel(aes(label=WeekSubWeek, color = factor(Weeks)),
  size = 3,
  arrow = arrow(length = unit(0.005, 'npc'), type = "closed"),
  force = 0.5,
  point.padding = unit(0.5, 'lines'),
  max.iter = 2e3,
  nudge_x = .05)
#ylab(expression(paste({delta}^13,"C", ' \u211')))
#ylab(expression(paste({delta}^13,"C")))

```

iso



```

ggsave(iso, filename = "Outlet_Delta_ti_cont.png", width = 8, height = 5, units = "in", scale = 1)

```

```

# DeltaDelta Water

```

```

#limits_DdCwater <- aes(ymin=diss.d13C-SD.d13C-initialDelta, ymax=diss.d13C+SD.d13C-initialDelta, color = factor(Weeks))
limits_DdCwater <- aes(ymin=diss.d13C-se.d13C-initialDelta, ymax=diss.d13C+se.d13C-initialDelta, color = factor(Weeks))

```

```

iso2 <- ggplot(A0df, aes(x=ti, y=DD13C.diss)) +
  # Error bars
  # geom_errorbar(aes(ymin=mean.d13C-SD.d13C, ymax=mean.d13C+SD.d13C), width=.1) +
  geom_errorbar(limits_DdCwater, width=1) +

```

```

# Themes and Axes
# theme_gray() +

```

```

# theme(axis.text.x = element_blank()) +
# theme(plot.margin = unit(c(1,1,1,1), "lines")) +
theme_bw() +
theme(legend.position="none",
      # legend.title = element_blank(),
      axis.text.x=element_text(angle = 45, hjust = 1)) +
guides(col = guide_legend(nrow = 2)) + # Sets legend parameters
xlab("Date") +
scale_x_datetime(breaks = date_breaks("2 weeks"), labels = date_format("%b %d")) +

# scale_y_continuous(breaks = c(-32,-31,-30,-29, -28, -27), limits = c(-32, -26.4) ) +
# scale_y_continuous(breaks = c(6, 4, 2, 0), limits = c(-1, 6) ) +
scale_y_continuous(breaks=seq(0, 6, 1)) +
ylab(expression(paste({Delta}, {delta}^"13", "C", ' (\u2030)')) +

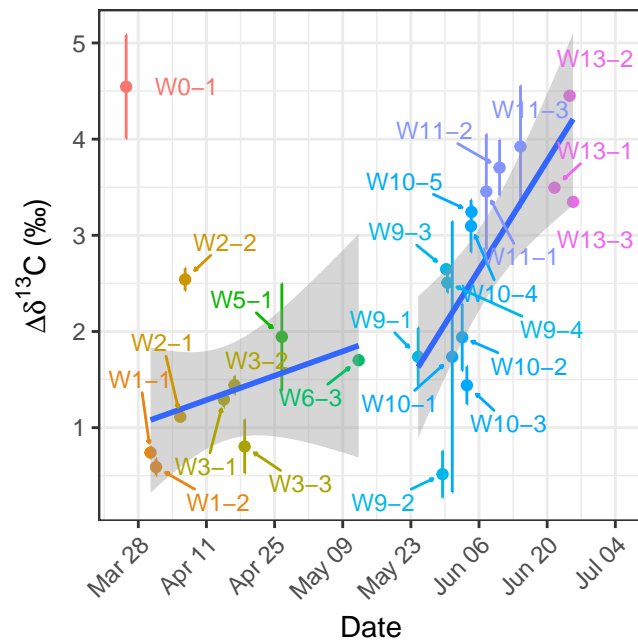
#scale_x_datetime(breaks = date_breaks("week"), labels = date_format("%m/%d")) +
geom_point( aes(color = Weeks, group = Weeks)) +

# Smooth linear models
# stat_smooth(method = "lm", formula = y ~ x) +
# geom_smooth(data=subset(AOdf[4:length(AOdf), ]), method = "lm", formula = y ~ poly(x, 2)) +
geom_smooth(data=subset(AOdf[4:27, ]), method = "lm", formula = y~x) +
geom_smooth(data=subset(AOdf[28:length(AOdf), ]), method = "lm", formula = y ~ x) +

# Text
# annotate("text",
#         x = as.POSIXct('2016-06-10 08:04:00'), y = 0.3, label = lbW9, parse = T, size = 3.0) +
# geom_segment(aes(x = as.POSIXct('2016-06-05 08:04:00'), y = 0.2,
#                 xend = as.POSIXct('2016-05-25 18:04:00'), yend = 0), color = "black",
#             arrow = arrow(length = unit(0.2, "cm")))) +
# annotate("text", x = as.POSIXct('2016-06-25 00:04:00'), y = -31.2, label = lb1, parse = T) +
geom_text_repel(aes(label=WeekSubWeek, color = factor(Weeks)),
               size = 3,
               arrow = arrow(length = unit(0.005, 'npc'), type = "closed"),
               force = 0.5,
               point.padding = unit(0.5, 'lines'),
               max.iter = 2e3,
               nudge_x = .05)
#ylab(expression(paste({delta}^"13", "C", ' \211'))))
#ylab(expression(paste({delta}^"13", "C")))

```

iso2



```
# plot_grid(co, deltaTime, ncol = 1, nrow = 2, align = "v")
```

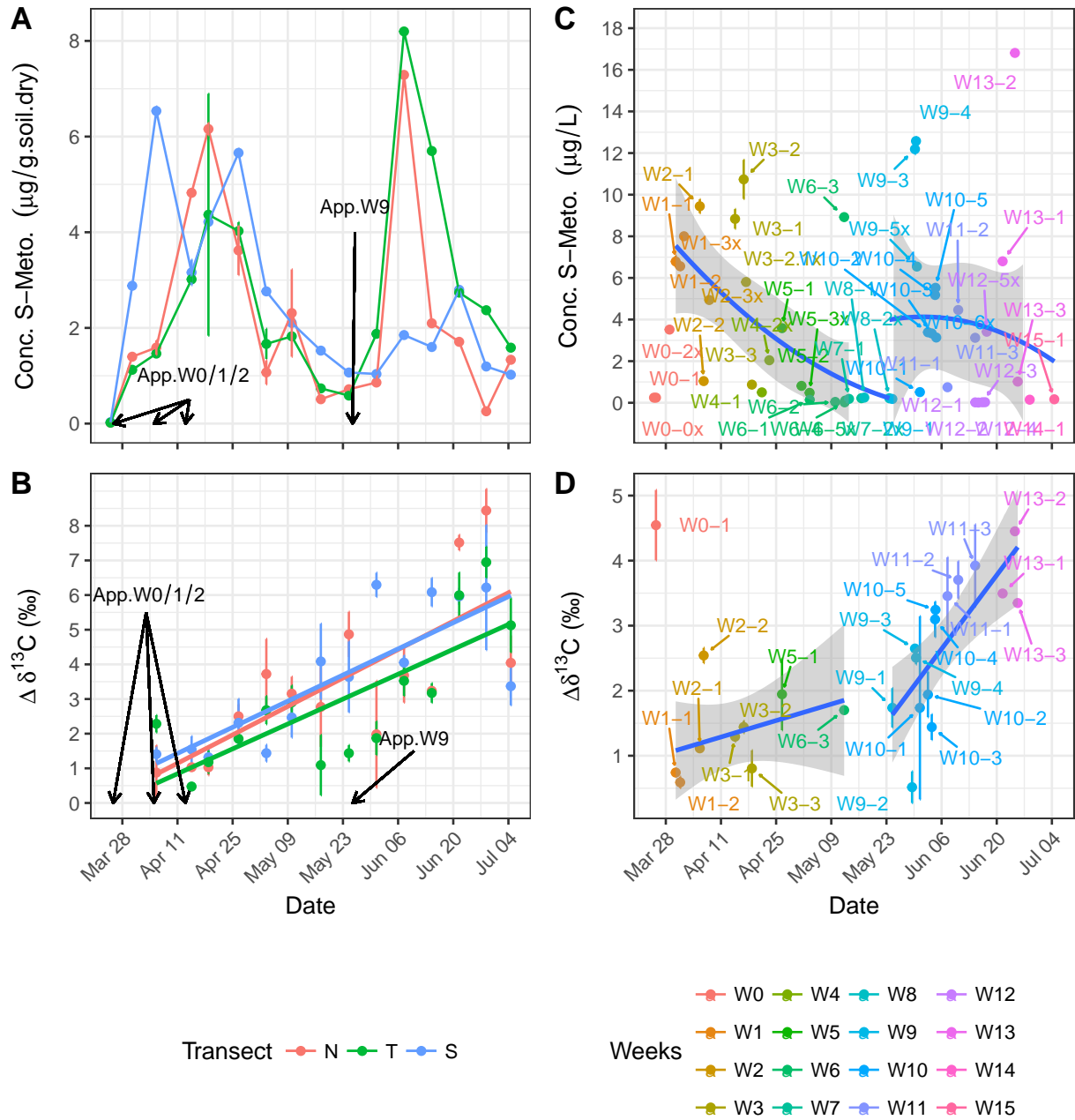
All plots

```
concSoils <- co + theme(legend.position='none')
concWater <- conc1 + theme(legend.position='none')

legend_soils = get_legend(co)
legend_water = get_legend(conc1)

grid4 <- plot_grid(concSoils, concWater, deltaTime, iso2,
                    ncol =2, nrow = 2, align ="v",
                    labels = c("A", "C", "B", "D"))
fig1 <- ggdraw() +
  draw_plot(grid4, x=0, y=.2, width = 1, height = .8) +
  draw_plot(legend_water, x=0.5, y = 0, width = 0.5, height = 0.2) +
  draw_plot(legend_soils, x=0, y=0, width = 0.6, height = 0.2)

fig1
```



```
ggsave(fig1, filename = "SoilsAndOutlet.tiff", height = 18, width = 17.8, units = 'cm')
```

Mass balance approach

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

soilsOut = read.csv2("Data/MassBalance_R.csv", header = T)
```

```

soilsOut$ti <- as.POSIXct(soilsOut$ti, "%Y-%m-%d %H:%M", tz = "EST")
sum(is.na(soilsOut$ti))

## [1] 0

print("Mass Balance Soils")

## [1] "Mass Balance Soils"

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/ 17 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/ 17 levels "AW-T-0","AW-T-0x",...: 2 NA NA 1 NA NA 3 NA NA 10 ...
## $ 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/ 17 levels "AW-S-0","AW-S-0x",...: 2 NA NA 1 NA NA 3 NA NA 10 ...
## $ 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 ...

# 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)

##Then rearrange your data frame
remainMassMolten <- soilsRemainMass[, c("ti", "CumAppMass.g", "CumOutDiss.g", "CumOutFilt.g", "CumOutMELsm.g")]
remainMassMolten <- melt(remainMassMolten, id=c("ti"))

# View(remainMassMolten)

pg <- remainMassMolten
pg <- na.omit(pg)

# 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"] <- "Persistent SM (Top soil 1cm)"

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] "Persistent SM (Top soil 1cm)"

pg$variable <- factor(pg$variable, levels = c("Applied SM Cum. (Survey)", "Persistent SM (Top soil 1cm)", "Dissolved SM Cum. (Outlet)", "Sediment SM Cum. (Outlet)", "MEL-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)) +
  geom_point(aes(x=ti, y=value, group = variable, shape=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(group = "Estimated Mass") +
  guides(col = guide_legend(ncol = 1)) + # Sets legend parameters
  scale_colour_manual(values=c("black", "dodgerblue4", "violet", "chartreuse4", "sandybrown")) +
  scale_shape_manual(values = c(8, 17, 25, 18, 7)) +

  #scale_colour_manual(values=c("black", "chartreuse4", "orangered2", "#F8766D", "dodgerblue4", "#619EED")) +
  #scale_shape_manual(values = c(15, 18, 16, 23, 17, 13, 6)) +

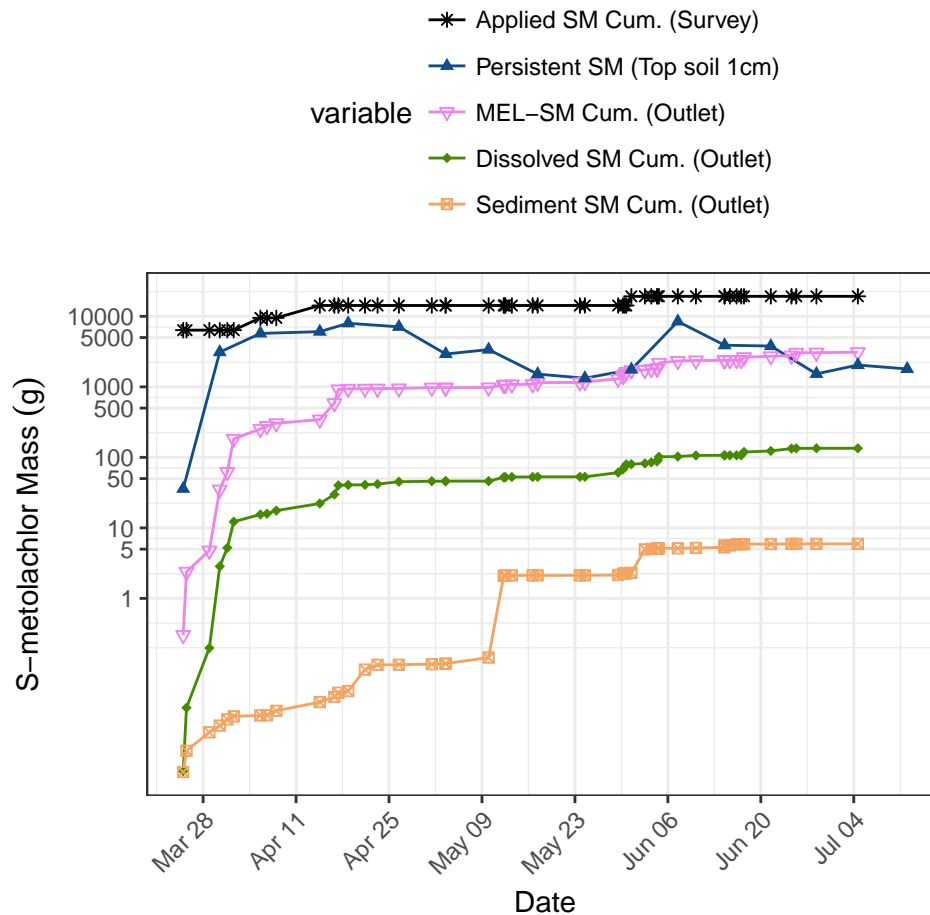
  xlab("Date") +

```

```

scale_x_datetime(breaks = date_breaks("2 weeks"), labels = date_format("%b %d")) +
ylab(expression(paste("S-metolachlor 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")

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("S-metolachlor ", {(g)})))

# massBal_MEL

massBalLegend <- get_legend(massBalTop)

```

Catchment degradation based on bulk signatures

```

# Pure and cuve isotope average
d13Co = -31.2144

# Lab enrichment:
# Alteck
# More degr. under saturation because anaerobic is best according to Fatima
epsilon_max = -1.5 # +/- 0.3 (@ 20C, 20% vwc)
epsilon_min = -2.0 # +/- 0.2 (@ 20C, 40% vwc)

epsilon_mean = -1.75

# Vine
# (@ 20C, 20% vwc) -0.8 +/- 0.1
# (@ 30C, 20% vwc) -1.4 +/- 0.2
# (@ 20C, 40% vwc) -1.7 +/- 0.2
# Average

# Remaining fraction
soilsOut$DD13C.bulk <- (soilsOut$BulkCatch.d13 - (d13Co))

# Max epsilon (30C, 20%)
soilsOut$f.max.bulk <-

```



```

((10^(-3)*soilsOut$BulkCatch.d13 + 1)/(10^(-3)*d13Co + 1))^(1000/(epsilon_max))

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

# Min epsilon (20C, 40%)
soilsOut$f.min.bulk <-
  ((10^(-3)*soilsOut$BulkCatch.d13 + 1)/(10^(-3)*d13Co + 1))^(1000/(epsilon_min))

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

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

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

bulkB <- ggplot(soilsOut, aes(x=ti, y=B.mean.bulk)) +
  geom_point() +
  # geom_point(aes(x=Date.ti, y=B.comp, colour=Transect, group = Transect)) +

# Theme and axes
theme_bw() +
ylab("Degr. %") +
theme(legend.position = "top",
      #axis.title = element_blank(),
      #axis.title.x = element_blank(),
      #axis.text.x = element_blank()
      axis.text.x=element_text(angle = 45, hjust = 1)
    ) +
xlab("Date") +
scale_x_datetime(breaks = date_breaks("2 weeks"), labels = date_format("%b %d")) +

# scale_y_continuous(breaks = c(25, 50, 75, 100), limits = c(0, 100) ) +
# stat_smooth(method = "lm", formula = y ~ poly(x, 2), se=FALSE)
# geom_smooth(data=subset(weeklySoil[14:28, ]), method = "lm", formula = y ~ poly(x, 2), se = F) +
geom_smooth(aes(group = 1), method = "lm", formula = y ~ poly(x, 2))
# stat_smooth(data=subset(weeklySoil[4:39, ]), method = "lm", formula = y ~ poly(x, 2), se = F)
# stat_smooth(method = "lm", formula = y ~ x, se=FALSE)
#geom_text_repel(aes(label=Wnum, color = factor(Transect)),
#  #
#    size = 3,
#  #
#    arrow = arrow(length = unit(0.005, 'npc'), type = "closed"),
#  #
#    force = 0.5,
#  #
#    point.padding = unit(0.5, 'lines'),
#  #
#    max.iter = 2e3,
#  #
#    nudge_x = .05)

# bulkB

```

Degradation based on transect signatures

```
# Merge Bulk Degradation into weekly soil dataframe (only one (e.g. South) transect as root)
soilsOut$PersistPrct <- (soilsOut$CatchMassSoil.g/soilsOut$CumAppMass.g)*100
soilsOut$DischPrct <- ((soilsOut$CumOutDiss.g+soilsOut$CumOutFilt.g)/soilsOut$CumAppMass.g)*100
bulkDegDF <- soilsOut[, c("ti", "WeekSubWeek", "ID.S", "BulkCatch.d13", "B.mean.bulk", "B.max.bulk", "B.min.bulk")]

bulkDegDF$TotBL <- bulkDegDF$B.min.bulk + bulkDegDF$PersistPrct + bulkDegDF$DischPrct
bulkDegDF$LeachPrct <- 100-bulkDegDF$TotBL
bulkDegDF$LeachPrctCorr <- ifelse(bulkDegDF$LeachPrct > 0, bulkDegDF$LeachPrct, NA)

# Delete rows from specified Columns
completeFun <- function(data, desiredCols) {
  completeVec <- complete.cases(data[, desiredCols])
  return(data[completeVec, ])
}

bulkDegDF <- completeFun(bulkDegDF, "TotBL")

bulkDegDF$Transect <- "Degraded (Bulk)"

# names(bulkDegDF)[names(bulkDegDF) == "B.mean.bulk"] <- "B.mean.com"
names(bulkDegDF)[names(bulkDegDF) == "ti"] <- "Date.ti"

# Splitting the identifier name into Type, Week No., tc..
bulkDegDF$ID.S <- as.character(bulkDegDF$ID.S)
split <- strsplit(bulkDegDF$ID.S, "AW-S-", fixed = T)
bulkDegDF$Wnum <- sapply(split, "[", 2) # Creates new column without "Split0"

bulkDegDF$Week = paste("W", bulkDegDF$Wnum, sep = "")

bulkDegDF <- bulkDegDF[, c("Date.ti", "Transect",
                          "B.mean.bulk", "B.max.bulk", "B.min.bulk",
                          "PersistPrct", "DischPrct", "TotBL", "LeachPrct", "LeachPrctCorr",
                          "Week")]

bulkDegDF$RemainLabel <- "Persistent frac. (Top Soil 1cm)"
bulkDegDF$DischLabel <- "Discharge (Outlet)"
bulkDegDF$LeachLabel <- "Leached (Inferred)"

levels(bulkDegDF$Transect)[levels(bulkDegDF$Transect)=="Bulk"] <- "Degraded (Bulk)"

wSoil <- weeklySoil[, c("Date.ti", "Transect", "B.mean.comp", "B.max.comp", "B.min.comp")]
levels(wSoil$Transect)[levels(wSoil$Transect)=="N"] <- "North"
levels(wSoil$Transect)[levels(wSoil$Transect)=="T"] <- "Talweg"
levels(wSoil$Transect)[levels(wSoil$Transect)=="S"] <- "South"

# colnames(wSoil) <- c("Date.ti", "Transect", "B.mean.bulk", "B.max.bulk", "B.min.bulk")

# wSoil$Week <- NA
```

```

# wSoilBulkDeg <- rbind(wSoil, bulkDegDF)

#names(bulkDegDF)[names(bulkDegDF) == "ID.S"] <- "ID"
#wSoilBulkDeg <- merge(weeklySoil, bulkDegDF, by="ID", all = T)
#wSoilBulkDeg$BulkLabel[!is.na(wSoilBulkDeg$WeekSubWeek)] <- "Bulk"

levels(wSoil$Transect)

## [1] "North" "Talweg" "South"

#wSoil$Transect <- factor(wSoil$Transect, levels = c("Bulk Fraction", "North", "Talweg", "South" ))
wSoil$Transect <- factor(wSoil$Transect, levels = c("North", "Talweg", "South" ))

#wSoilBulkDeg$B.max.bulk[wSoilBulkDeg$Transect == "North"] <- NA
#wSoilBulkDeg$B.max.bulk[wSoilBulkDeg$Transect == "Talweg"] <- NA
#wSoilBulkDeg$B.max.bulk[wSoilBulkDeg$Transect == "South"] <- NA

#wSoilBulkDeg$B.min.bulk[wSoilBulkDeg$Transect == "North"] <- NA
#wSoilBulkDeg$B.min.bulk[wSoilBulkDeg$Transect == "Talweg"] <- NA
#wSoilBulkDeg$B.min.bulk[wSoilBulkDeg$Transect == "South"] <- NA

limits_bulkdeg <- aes(ymin=B.min.bulk, ymax=B.max.bulk, x = Date.ti, colour = Transect, group = Transect)

Bsoil1 <-
  ggplot() +
    # geom_point(size = 2) +
    # ggplot(data = wSoilBulkDeg, aes(Date.ti, B.mean.bulk, colour = Transect, shape=Transect, group = Transect)) +
    geom_point(data = wSoil,
               aes(Date.ti, B.mean.comp, colour = Transect, shape=Transect, group = Transect), size = 2) +
    geom_point(data = bulkDegDF,
               aes(Date.ti, B.mean.bulk, colour = Transect, shape=Transect, group = Transect), size = 2) +
    geom_point(data = bulkDegDF,
               aes(Date.ti, PersistPrct, colour = RemainLabel, shape=RemainLabel, group = RemainLabel), size = 2) +
    geom_point(data = bulkDegDF,
               aes(Date.ti, DischPrct, colour = DischLabel, shape=DischLabel, group = DischLabel), size = 2) +
    geom_point(data = bulkDegDF,
               aes(Date.ti, LeachPrctCorr, colour = LeachLabel, shape=LeachLabel, group = LeachLabel), size = 2) +

    geom_errorbar(data = bulkDegDF, limits_bulkdeg) + # With 2 data frames
    stat_smooth(data=subset(bulkDegDF, Transect == "Degraded (Bulk)"),
                mapping = aes(y = B.mean.bulk, x = Date.ti), # With 2 data frames
                colour = "black",
                method = "lm", formula = y ~ poly(x, 2), se=F) +

    stat_smooth(data=subset(bulkDegDF, RemainLabel == "Persistent frac. (Top Soil 1cm)"),
                mapping = aes(y = PersistPrct, x = Date.ti), # With 2 data frames
                colour = "darkblue",
                method = "lm", formula = y ~ poly(x, 2), se=F) +
    scale_colour_manual(values=c("black", "chartreuse4", "orangered2", "#F8766D", "dodgerblue4", "#619EED")) +
    scale_shape_manual(values = c(15, 18, 16, 23, 17, 13, 6)) +
    theme_bw() +
    ylab("S-metolachlor Sinks (%)") +
    theme(legend.position = "top",

```

```

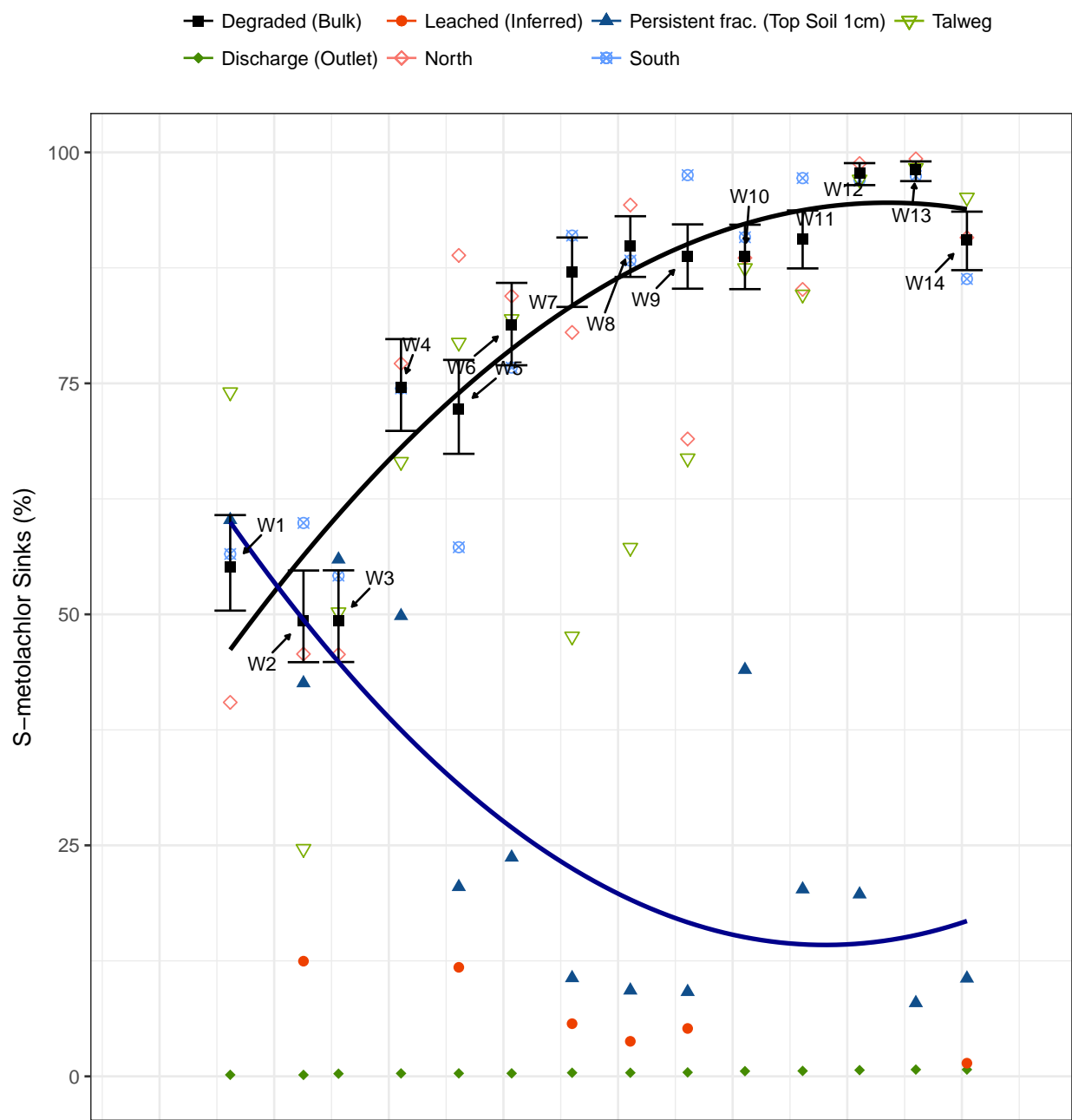
    legend.title = element_blank(),
    #axis.title = element_blank(),
    axis.title.x = element_blank(),
    axis.text.x = element_blank()
    #axis.text.x=element_text(angle = 45, hjust = 1)
  ) +
  # xlab("Date") +
  scale_x_datetime(breaks = date_breaks("2 weeks"), labels = date_format("%b %d")) +
  # ylab(expression(paste("Degradation %")))) +

  # scale_y_continuous(breaks = c(25, 50, 75, 100), limits = c(0, 100) ) +

  # geom_smooth(data=subset(weeklySoil[14:28, ]), method = "lm", formula = y ~ poly(x, 2), se = F) +
  # geom_smooth(aes(group = 1), method = "lm", formula = y ~ poly(x, 2)) +
  # stat_smooth(data=subset(weeklySoil[4:39, ]), method = "lm", formula = y ~ poly(x, 2), se = F)
  # stat_smooth(method = "lm", formula = y ~ x, se=FALSE)
  geom_text_repel(data=subset(bulkDegDF, Transect == "Degraded (Bulk)"),
    mapping = aes(y=B.mean.bulk, x= Date.ti, label=Week),
    size = 3,
    arrow = arrow(length = unit(0.005, 'npc'), type = "closed"),
    force = 0.9,
    point.padding = unit(0.9, 'lines'),
    max.iter = 2e3,
    nudge_x = .05, show.legend = F)

```

Bsoil1



```
colnames(bulkDegDF)[which(names(bulkDegDF) == "Transect")] <- "Catchment"
limits_bulkdegCAT <- aes(ymin=B.min.bulk, ymax=B.max.bulk, x = Date.ti, colour = Catchment, group = Cat
solidpts <- ggplot() +
  # geom_point(size = 2) +
  # ggplot(data = wSoilBulkDeg, aes(Date.ti, B.mean.bulk, colour = Transect, shape=Transect, group = Tr
  geom_point(data = bulkDegDF,
    aes(Date.ti, B.mean.bulk, colour = Catchment, shape=Catchment, group = Catchment), size = 2)
  geom_point(data = bulkDegDF,
    aes(Date.ti, PersistPrct, colour = RemainLabel, shape=RemainLabel, group = RemainLabel), size = 2)
  geom_point(data = bulkDegDF,
    aes(Date.ti, DischPrct, colour = DischLabel, shape=DischLabel, group = DischLabel), size = 2)
```

```

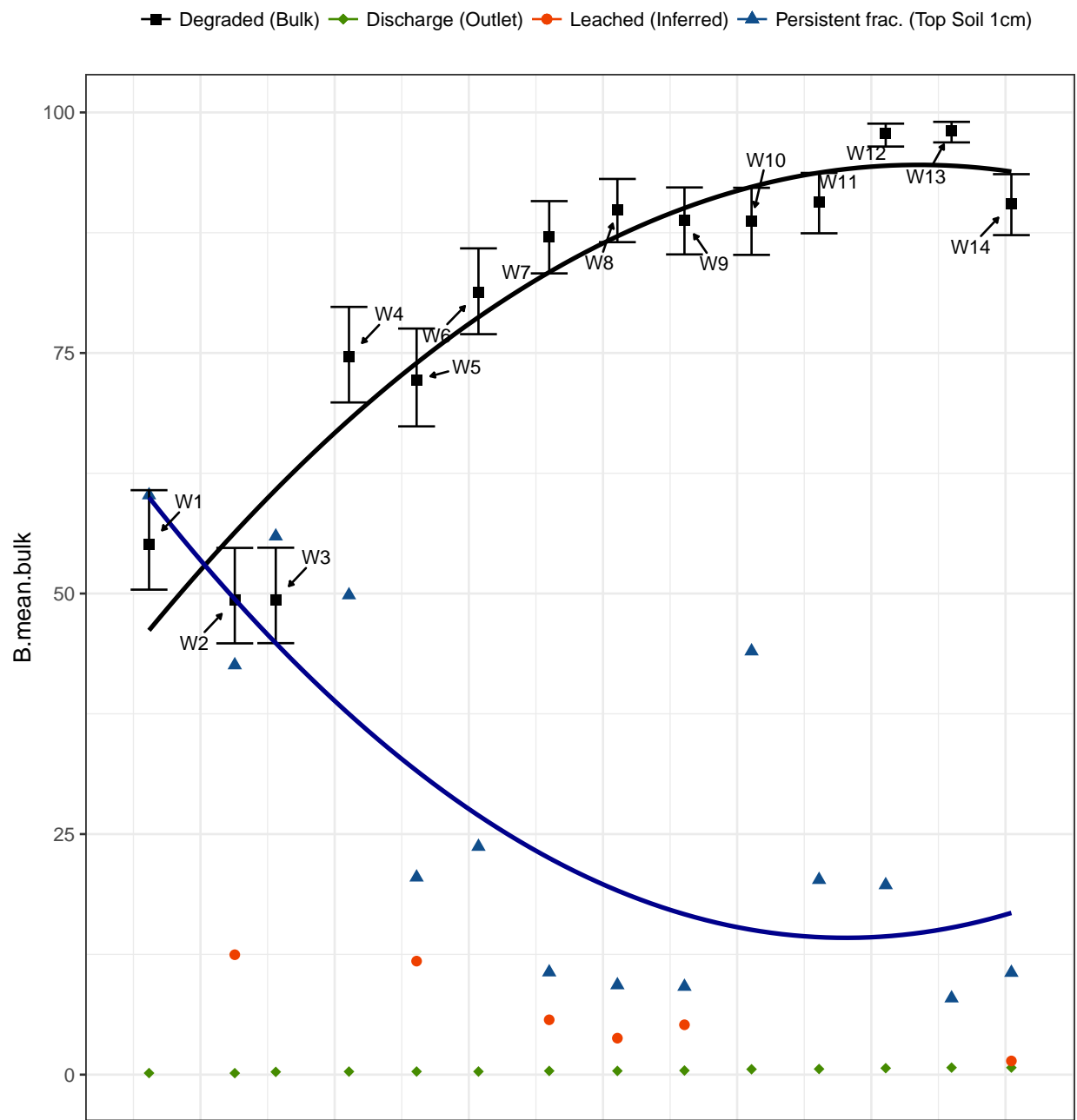
geom_point(data = bulkDegDF,
           aes(Date.ti, LeachPrctCorr, colour = LeachLabel, shape=LeachLabel, group = LeachLabel), si

geom_errorbar(data = bulkDegDF, limits_bulkdegCAT) + # With 2 data frames
stat_smooth(data=subset(bulkDegDF, Catchment == "Degraded (Bulk)"),
            mapping = aes(y = B.mean.bulk, x = Date.ti), # With 2 data frames
            colour = "black",
            method = "lm", formula = y ~ poly(x, 2), se=F) +

stat_smooth(data=subset(bulkDegDF, RemainLabel == "Persistent frac. (Top Soil 1cm)"),
            mapping = aes(y = PersistPrct, x = Date.ti), # With 2 data frames
            colour = "darkblue",
            method = "lm", formula = y ~ poly(x, 2), se=F) +
#scale_colour_manual(values=c("black", "#F8766D", "#7CAE00", "#619CFF")) +
scale_colour_manual(values=c("black", "chartreuse4", "orangered2", "dodgerblue4")) +
scale_shape_manual(values = c(15, 18, 16, 17)) +
theme_bw() +
theme(legend.position = "top",
      legend.title = element_blank(),
      #axis.title = element_blank(),
      axis.title.x = element_blank(),
      axis.text.x = element_blank()
      #axis.text.x=element_text(angle = 45, hjust = 1)
      ) +
# xlab("Date") +
scale_x_datetime(breaks = date_breaks("2 weeks"), labels = date_format("%b %d")) +
geom_text_repel(data=subset(bulkDegDF, Catchment == "Degraded (Bulk)"),
               mapping = aes(y=B.mean.bulk, x= Date.ti, label=Week),
               size = 3,
               arrow = arrow(length = unit(0.005, 'npc'), type = "closed"),
               force = 0.9,
               point.padding = unit(0.9, 'lines'),
               max.iter = 2e3,
               nudge_x = .05, show.legend = F)

solidpts

```



```

#colnames(wSoil)[which(names(wSoil) == "Transect")] <- "Transect-Deg."
emptypts <-
  ggplot() +
    # geom_point(size = 2) +
    # ggplot(data = wSoilBulkDeg, aes(Date.ti, B.mean.bulk, colour = Transect, shape=Transect, group = Transect)) +
    geom_point(data = wSoil,
               aes(Date.ti, B.mean.comp, colour = Transect, shape=Transect, group = Transect), size = 2)

#scale_colour_manual(values=c("black", "#F8766D", "#7CAE00", "#619CFF")) +

scale_colour_manual(values=c("#F8766D", "#7CAE00", "#619CFF")) +

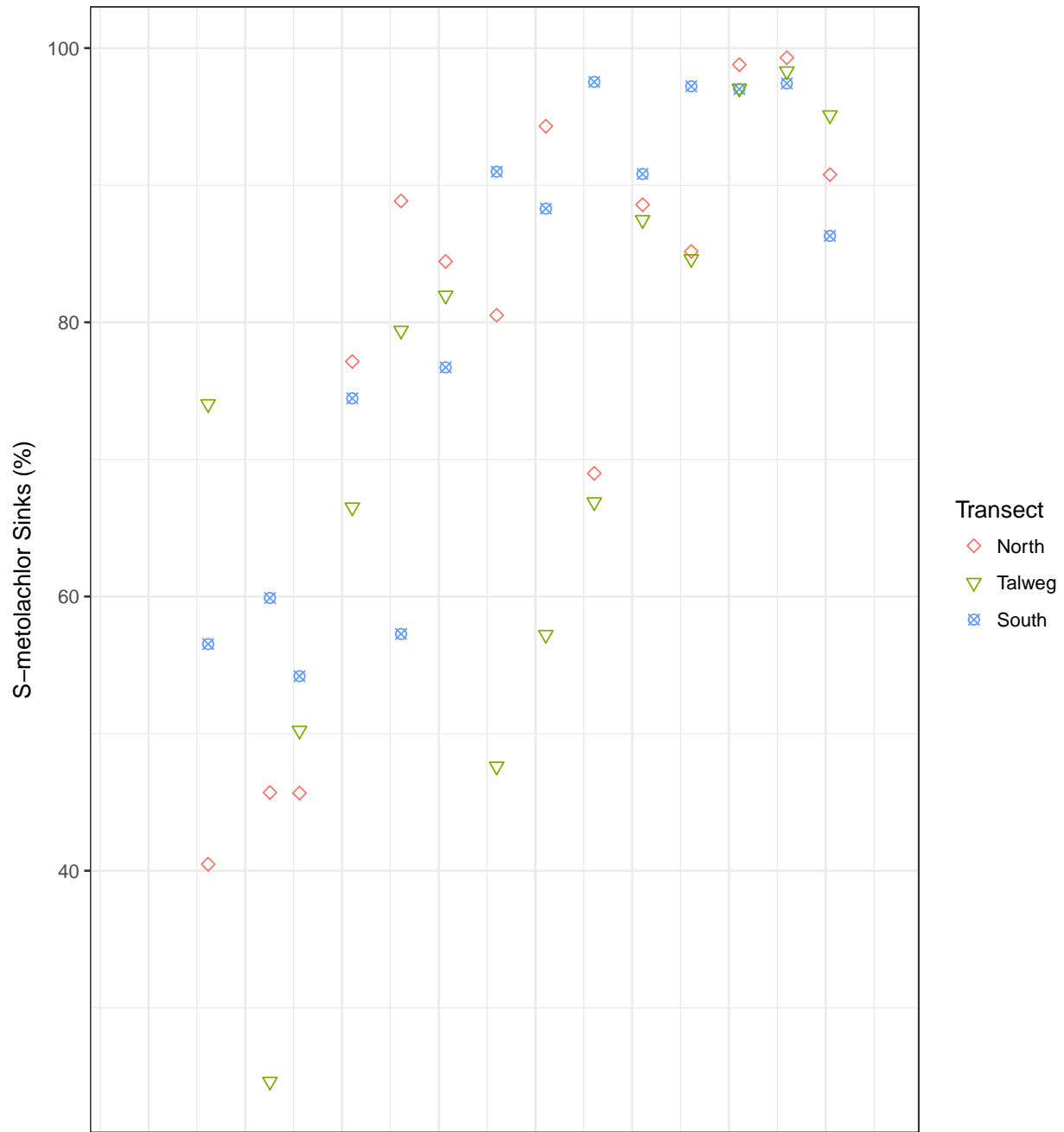
```

```

scale_shape_manual(values = c(23, 6, 13)) +
# guides(guide_legend(title = waiver()))+
# labs(color = "Number of gears") +
#scale_colour_manual(values=c("black" , "chartreuse4", "orangered2", "#F8766D", "dodgerblue4", "#61
#scale_shape_manual(values = c(15, 18, 16, 23, 17, 13, 6)) +
theme_bw() +
ylab("S-metolachlor Sinks (%)") +
theme(#legend.position = "top",
      # legend.title = element_blank(),
      #axis.title = element_blank(),
      axis.title.x = element_blank(),
      axis.text.x = element_blank()
      #axis.text.x=element_text(angle = 45, hjust = 1)
      ) +
# xlab("Date") +
scale_x_datetime(breaks = date_breaks("2 weeks"), labels = date_format("%b %d"))

emptypts

```

```
#colnames(wSoil)[which(names(wSoil) == "Transect-Deg.")] <- "Transect"

## Merging both figures

# massBalNoL <- massBal + theme(legend.position='none')
BsoilNoL <- Bsoil1 + theme(legend.position='none')
MBalNoL <- massBalTop + theme(legend.position = 'none')

legend_deg_solid = get_legend(solidpts +
  theme(legend.title = element_text(face = "bold"),
    legend.text = element_text(size = 9),
```

```

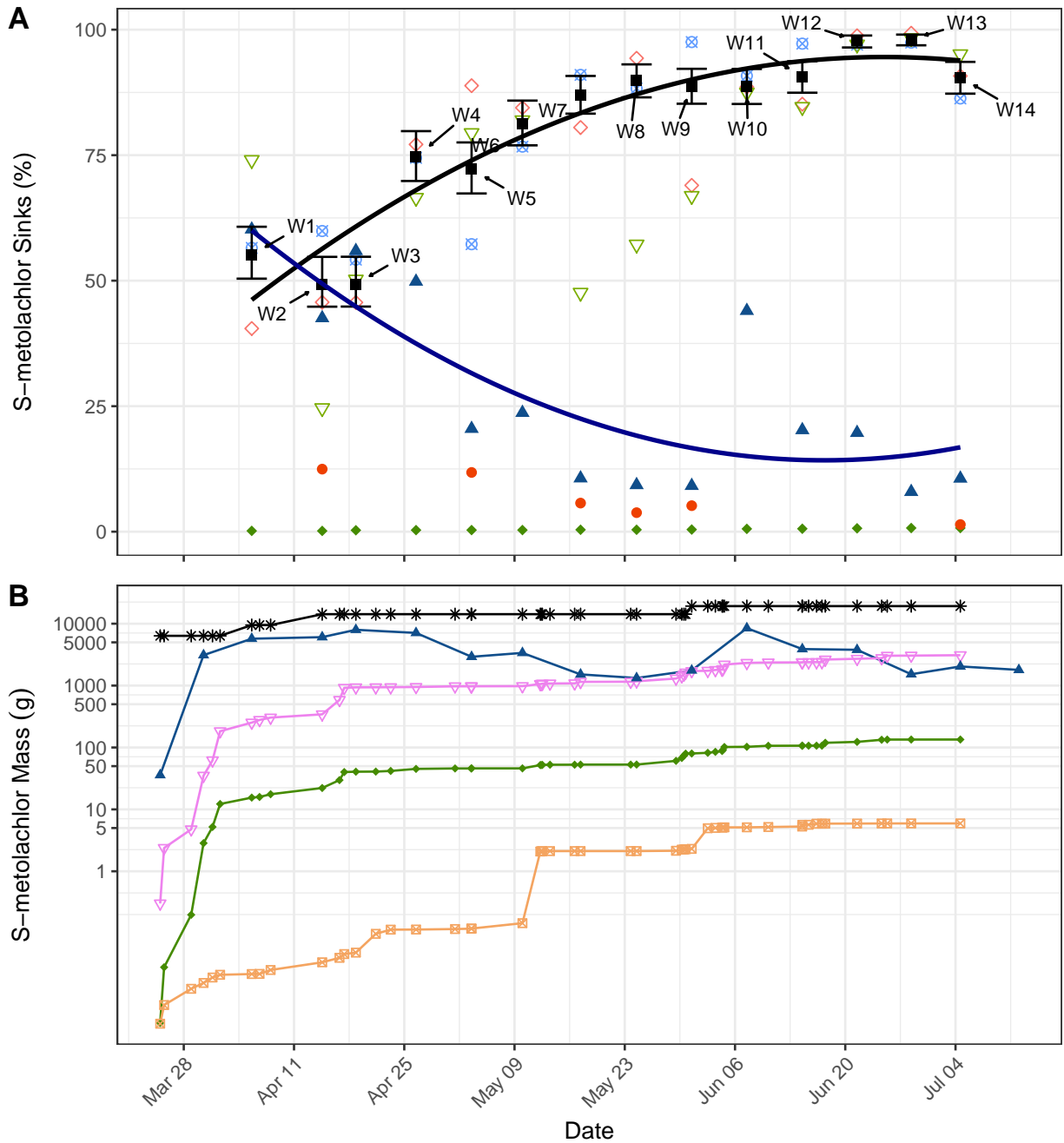
        legend.key.height = unit(x = 0.35, units = 'cm'),
        legend.background = element_rect(colour = "black")) +
        guides(colour = guide_legend(title.position = "top", ncol = 1, byrow = T)))

legend_deg_empty = get_legend(emptypts +
    theme(legend.title = element_text(face = "bold"),
          legend.text = element_text(size = 9),
          legend.key.height = unit(x = 0.35, units = 'cm'),
          legend.background = element_rect(colour = "black")) +
    guides(colour = guide_legend(title.position = "top", ncol = 1, byrow = T)))

legend_mass = get_legend(massBalTop +
    theme(legend.text = element_text(size = 9),
          legend.key.height = unit(x = 0.4, units = 'cm'),
          legend.background = element_rect(colour = "black"),
          legend.title = element_blank()))
    #+ guides(colour = guide_legend(title = "Mass Distribution", title.position

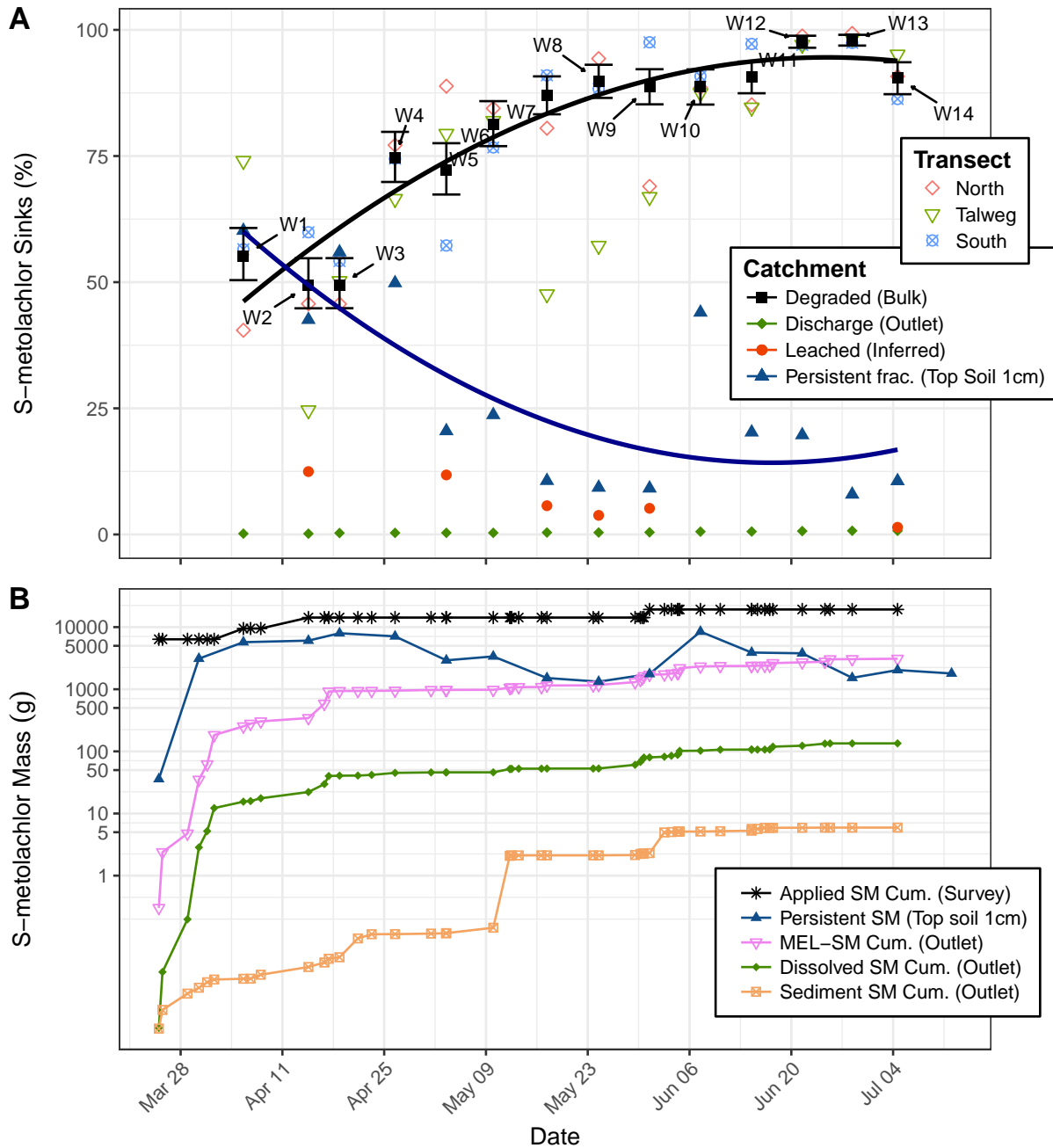
gridPartB <- plot_grid(BsoilNoL, MBalNoL,
    ncol = 1, nrow = 2, align = "v",
    labels = c("A", "B"))
gridPartB

```



```
fig2 <- ggdraw() +
  draw_plot(gridPartB, x=0, y=0, width = 0.93, height = 1) +
  draw_plot(legend_deg_solid, x=0.48, y =0.62, width = 0.70, height = 0.20) +
  draw_plot(legend_deg_empty, x=0.52, y =0.65, width = 0.75, height = 0.35) +
  draw_plot(legend_mass, x=0.5, y=0.05, width = 0.63, height = 0.28)
```

fig2



```
ggsave(fig2, filename = "BvsMassBal.tiff", height = 17, width = 17.8, units = 'cm')
```

Degradation per transect (no bulk)

```
Bsoil2 = ggplot(wSoil, aes(x=Date.ti, y=B.mean.comp, colour=Transect, shape=Transect, group = Transect)) +
  # Bsoil2 = ggplot(wSoilBulkDeg, aes(x=Date.ti)) +
  #
  # stat_smooth(aes(y=B.mean.bulk), method = "lm", formula = y ~ poly(x, 2), se=T) +
  # geom_point(aes(y=B.mean.com, colour=Transect, group = Transect)) +
  # geom_point(aes(y=B.mean.bulk, group=BulkLabel, colour="Bulk Isotopes")) +
```

```

geom_point(size = 2) +

stat_smooth( method = "lm", formula = y ~ poly(x, 2), se=F) +

scale_colour_manual(values=c("#F8766D", "#7CAE00", "#619CFF")) +
scale_shape_manual(values = c(15, 16, 17)) +
# scale_shape_manual(values = c(23, 15, 16, 17)) +
# geom_point(aes(x=Date.ti, y=B.comp, colour=Transect, group = Transect)) +
# Theme and axes
theme_bw() +
ylab("Degr. %") +
theme(legend.position = "top",
      #axis.title = element_blank(),
      axis.title.x = element_blank(),
      axis.text.x = element_blank()
      #axis.text.x=element_text(angle = 45, hjust = 1)
      ) +
# xlab("Date") +
scale_x_datetime(breaks = date_breaks("2 weeks"), labels = date_format("%b %d"))
# ylab(expression(paste("Degradation %")))) +

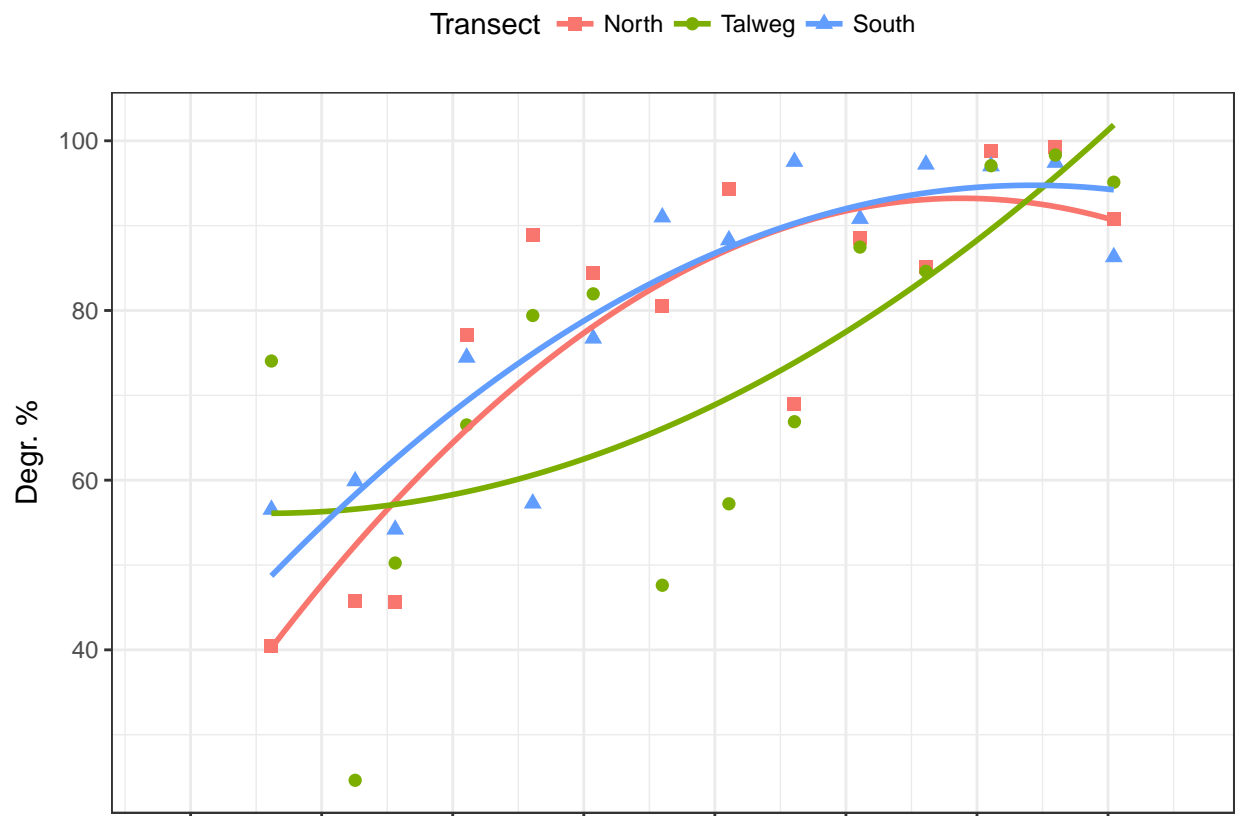
# scale_y_continuous(breaks = c(25, 50, 75, 100), limits = c(0, 100) ) +

# geom_smooth(data=subset(weeklySoil[14:28, ]), method = "lm", formula = y ~ poly(x, 2), se = F) +
# geom_smooth(aes(group = 1), method = "lm", formula = y ~ poly(x, 2)) +
# stat_smooth(data=subset(weeklySoil[4:39, ]), method = "lm", formula = y ~ poly(x, 2), se = F)
# stat_smooth(method = "lm", formula = y ~ x, se=FALSE)

#geom_text_repel(aes(y=B.mean.bulk, label=Wnum, color = factor(Transect)),
#               size = 3,
#               arrow = arrow(length = unit(0.005, 'npc'), type = "closed"),
#               force = 0.5,
#               point.padding = unit(0.5, 'lines'),
#               max.iter = 2e3,
#               nudge_x = .05)

```

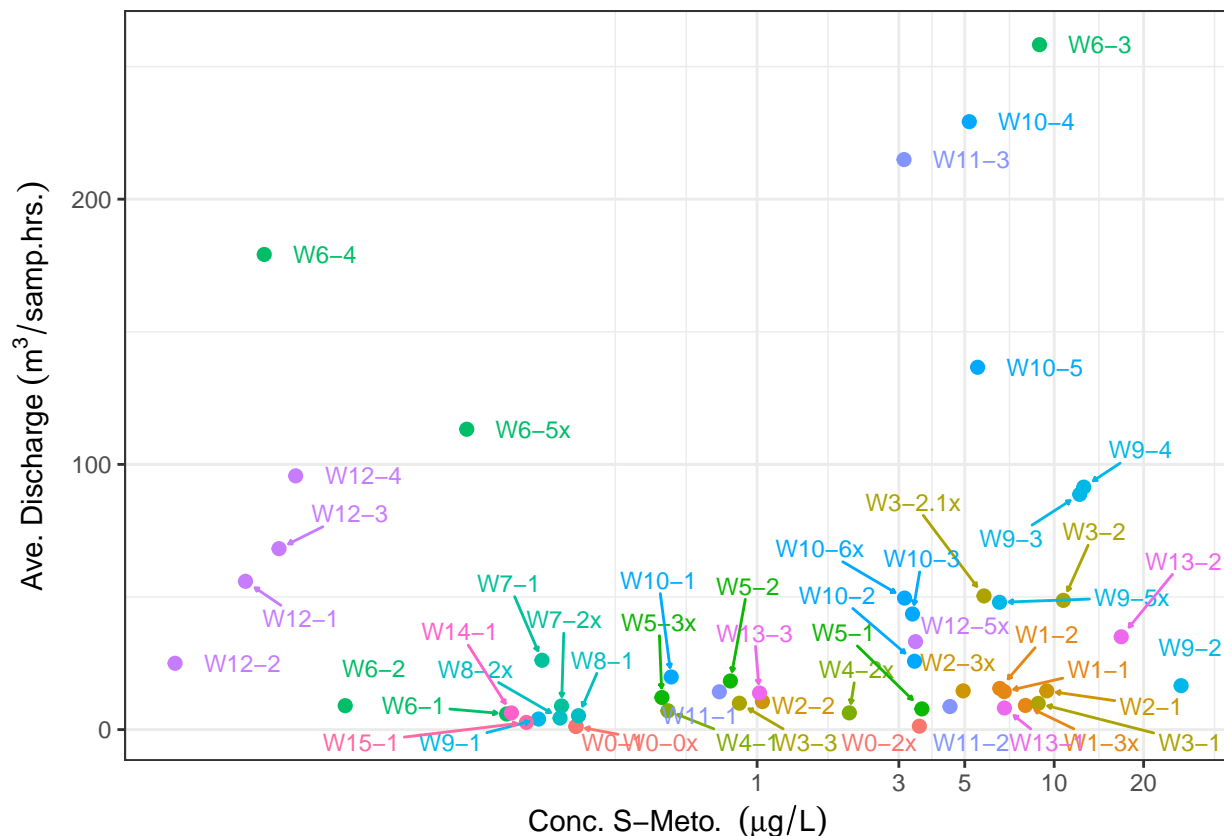
Bsoil2



XY-Plots

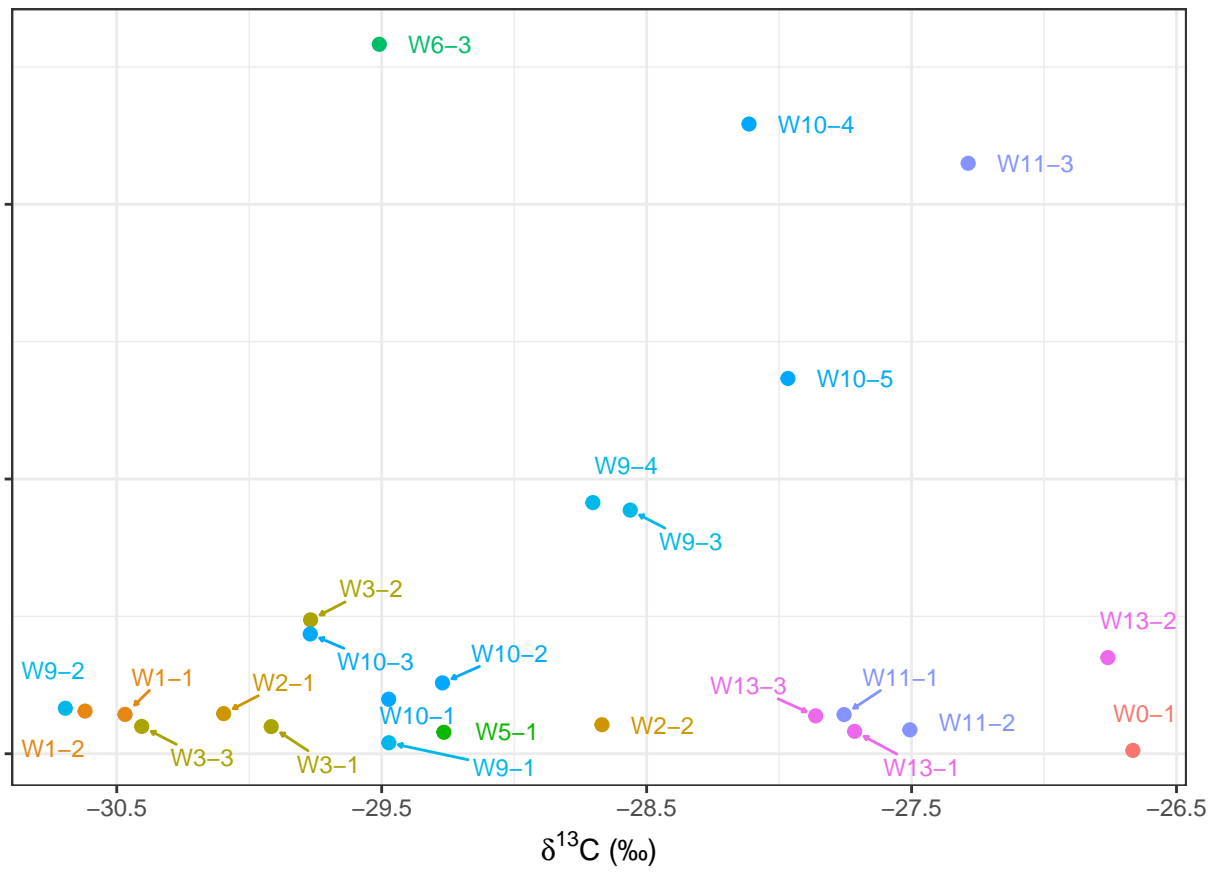
```
QC <- ggplot(A0df, aes(y=AveDischarge.m3.h, x=Conc.mug.L, group = WeekSubWeek, color = Weeks)) +
  geom_point(size = 2) +
  theme_bw() +
  theme(axis.text.y = element_blank()) +
  theme(legend.title=element_blank()) +
  theme(plot.margin = unit(c(0,0.5,0,0), "lines")) +
  #stat_smooth(method = "lm", formula = y ~ poly(x, 2)) +
  theme_bw() +
  theme(legend.position="none") +
  #scale_y_continuous(trans=log_trans(), breaks=c(1, 5, 10, 50, 100, 200)) +
  scale_x_continuous(trans=log_trans(), breaks=c(1, 3, 5, 10, 20)) +
  ylab(expression(paste("Ave. Discharge ", {(m^3} / samp.hrs. )}))) +
  xlab(expression(paste("Conc. S-Meto. ", {(mu}*g / L)}))) +
  geom_text_repel(aes(label=WeekSubWeek, color = factor(Weeks)),
    size = 3,
    arrow = arrow(length = unit(0.005, 'npc'), type = "closed"),
    force = 0.5,
    point.padding = unit(0.5, 'lines'),
    max.iter = 2e3,
    nudge_x = .05)
```

QC

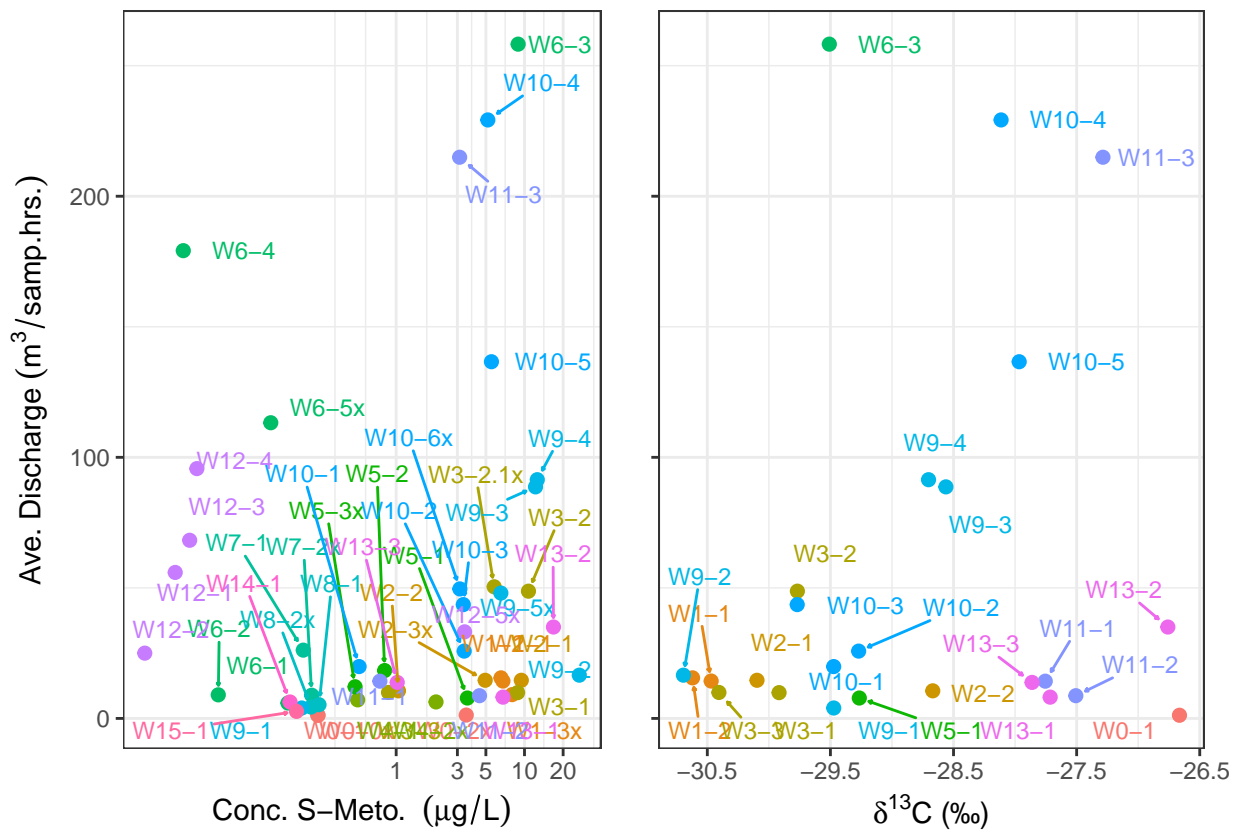


```
QD <- ggplot(A0df, aes(y=AveDischarge.m3.h, x=diss.d13C, group = WeekSubWeek, color = Weeks)) +
  geom_point(size = 2) +
  theme_bw() +
  theme(axis.text.y = element_blank()) +
  theme(plot.margin = unit(c(0,0.8,0,0), "lines")) +
  #theme(legend.title=element_blank()) +
  #theme(legend.text = element_text(size = 10)) +
  theme(legend.position="none") +
  #stat_smooth(method = "lm", formula = y ~ poly(x, 2)) +
  #scale_y_continuous(trans=log_trans(), breaks=c(1, 3, 5, 8, 10, 30, 50, 80, 100, 300)) +
  ylab(expression(paste("Ave. Discharge ", {(m^{3} / sample)}))) +
  ylab("") +
  scale_x_continuous(breaks=seq(-31.5, -26.5, 1)) +
  xlab(expression(paste({\delta}^{13}C, ' (‰)'))) +
  geom_text_repel(aes(label=WeekSubWeek, color = factor(Weeks)),
    size = 3,
    arrow = arrow(length = unit(0.005, 'npc'), type = "closed"),
    force = 0.5,
    point.padding = unit(0.5, 'lines'),
    max.iter = 2e3,
    nudge_x = .05)
```

QD



```
acd = plot_grid(QC, QD, ncol = 2, nrow = 1, align = "h")
acd
```

```
ggsave(acd, filename = "Disch_Conc_Delta_XYlabs.png", width = 8, height = 5, units = "in", scale = 1)
#ggsave(acd, filename = "Disch_Conc_Delta_XY.png", width = 8, height = 5, units = "in", scale = 1)
#ggsave(acd, filename = "Disch_Conc_Delta_W.pdf", width = 8, height = 4.6, units = "in", scale = 1)
```