Mass Soils - Composite Weeks Alteck 2016

PAZ

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Purpose

This file merges weekly composite concentrations and isotope data.

Imports:

- **SoilCompConc_W1toW15.csv**
- **SoilCompIsotopes_W1toW15.csv**

Generates:

- **MassIso_CompositeSoils.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"
```

Composite Concentrations & Isotope Data - Alteckendorf 2016

Isotopes selected where cleaned according to the following rules:

a) The isotope shift was not largely beyond (2x) Streitwieser theoretical limits (i.e. > 10)
b) Isotope shift was non-negative
c) Nanograms of carbon > 2.0.

1. Import CSV files

```
weeklySoilConc = read.csv2("Data/SoilCompConc_W1toW15.csv", header = TRUE)
weeklySoilConc$Date.ti <- as.POSIXct(strptime(weeklySoilConc$Date.Soil, "%d/%m/%Y %H:%M", tz="EST"))
sum(is.na(weeklySoilConc$Date.ti))
```

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

```
# View(weeklySoilConc)
weeklySoilConc <- weeklySoilConc[,c("Filename",
                                    "Transect",
                                    "Wnum",
```

```
                                    "Date.Soil",
                                    "Date.ti",
                                    "Conc.mug.g.dry.soil",
                                    "Conc.ComSoil.SD")]

colnames(weeklySoilConc)[colnames(weeklySoilConc) == "Filename"] <- "ID"
print("Soil Composites- Concentrations")
```

```
## [1] "Soil Composites- Concentrations"
```

```
str(weeklySoilConc)
```

```
## 'data.frame':    51 obs. of  7 variables:
##  $ ID                 : Factor w/ 51 levels "AW-N-0","AW-N-0x",..: 2 36 19 1 35 18 3 10 11 12 ...
##  $ Transect           : Factor w/ 3 levels "N","S","T": 1 3 2 1 3 2 1 1 1 1 ...
##  $ Wnum               : int  -1 -1 -1 0 0 0 1 2 3 4 ...
##  $ Date.Soil          : Factor w/ 17 levels "03/05/2016 13:10",..: 13 13 13 16 16 16 3 7 10 14 ...
##  $ Date.ti            : POSIXct, format: "2016-03-25 00:04:00" "2016-03-25 00:04:00" ...
##  $ Conc.mug.g.dry.soil: num  0.018 0.02 0.029 1.398 1.125 ...
##  $ Conc.ComSoil.SD    : num  NA NA NA NA NA ...
```

```
# weeklySoilIso = read.csv2("Data/SoilCompIsotopes_W1toW15.csv", header = TRUE) # JESIUM data (before n
weeklySoilIso  = read.csv2("Data/SoilCompIsotopes_W1toW15ng.csv", header = TRUE)

colnames(weeklySoilIso)[colnames(weeklySoilIso) == "DD13...31.21."] <- "DD13"
colnames(weeklySoilIso)[colnames(weeklySoilIso) == "ng..C."] <- "ngC"
colnames(weeklySoilIso)[colnames(weeklySoilIso) == "Filename"] <- "ID"

weeklySoilIso <- weeklySoilIso[, c("ID",
                                   "Repl",
                                   "d.13C.12C",
                                   "DD13",
                                   "ngC")]

weeklySoilIso <- subset(weeklySoilIso, DD13 > 0 & DD13 < 10 & ngC >= 2)


isoCompSummary = ddply(weeklySoilIso, c("ID"), summarise,
                       N_compsoil    = length(d.13C.12C),
                       comp.d13C = mean(d.13C.12C),
                       comp.d13C.SD = sd(d.13C.12C),
                       comp.d13C.SE = comp.d13C.SD / sqrt(N_compsoil))

print("Soil Composites - Isotopes All")
```

```
## [1] "Soil Composites - Isotopes All"
```

```
str(weeklySoilIso)
```

```
## 'data.frame':    126 obs. of  5 variables:
##  $ ID       : Factor w/ 42 levels "AW-N-1","AW-N-10",..: 1 1 2 2 3 3 7 7 7 8 ...
##  $ Repl     : int  2 3 1 3 1 3 1 2 3 1 ...
##  $ d.13C.12C: num  -31.1 -29.5 -28.3 -26.7 -27.8 ...
##  $ DD13     : num  0.087 1.664 2.898 4.464 3.382 ...
##  $ ngC      : num  3.82 3.62 7.07 8.34 9.21 ...
```

```r
print("Soil Composites - Isotopes Ave and St.Dev.")
```

```
## [1] "Soil Composites - Isotopes Ave and St.Dev."
```

```r
str(isoCompSummary)
```

```
## 'data.frame':    42 obs. of  5 variables:
##  $ ID          : Factor w/ 42 levels "AW-N-1","AW-N-10",..: 1 2 3 4 5 6 7 8 9 10 ...
##  $ N_compsoil  : int  2 2 2 3 3 3 3 3 2 3 ...
##  $ comp.d13C   : num  -30.3 -27.5 -28 -23.7 -22.8 ...
##  $ comp.d13C.SD: num  1.115 1.107 0.206 0.389 1.078 ...
##  $ comp.d13C.SE: num  0.789 0.783 0.146 0.224 0.622 ...
```

2. Merge lab concentrations and isotopes

```r
comp.CoIs = merge(weeklySoilConc, isoCompSummary, by = "ID", all = T)
comp.CoIs$Wnum = as.numeric(comp.CoIs$Wnum)
comp.CoIs <- comp.CoIs[order(comp.CoIs$Wnum),]
print("Merged Soil Concentrations and Isotopes")
```

```
## [1] "Merged Soil Concentrations and Isotopes"
```

```r
str(comp.CoIs)
```

```
## 'data.frame':    51 obs. of  11 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               : num  -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 ...
```

3. Compute Degradation Extent and Delta-delta

```r
# Pure and cuve isotope average
d13Co = -31.2144

# Lab enrichment:
# Alteck
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
comp.CoIs$DD13C.comp <- (comp.CoIs$comp.d13C - (d13Co))
```

```
# Max epsilon (30C, 20%)
comp.CoIs$f.comp <-
  ((10^(-3)*comp.CoIs$comp.d13C + 1)/(10^(-3)*d13Co + 1))^(1000/(epsilon_max))

comp.CoIs$B.comp <-
  (1 - comp.CoIs$f.comp)*100

# Min epsilon (20C, 40%)
comp.CoIs$f.min.comp <-
  ((10^(-3)*comp.CoIs$comp.d13C + 1)/(10^(-3)*d13Co + 1))^(1000/(epsilon_min))

comp.CoIs$B.min.comp <-
  (1 - comp.CoIs$f.min.comp)*100

# Mean epsilon (# Alteck)
comp.CoIs$f.mean.comp <-
  ((10^(-3)*comp.CoIs$comp.d13C + 1)/(10^(-3)*d13Co + 1))^(1000/(epsilon_mean))

comp.CoIs$B.mean.com <-
  (1 - comp.CoIs$f.mean.comp)*100
```

3. Compute Soil S-metolachlor Mass at time t across space

For non-measured plots, the soil concentration and isotope measured at the neareast transect is assumed. The total area for each transect is calculated and shown below.

The total pesticide mass for each transect at time t is then given by:

$$M(t)_{Ta} = C(t)_T \cdot \rho \cdot A_T \cdot D\cdot$$

```
# S-metolachlor Mass [g]
# Conc. [ug/g dry soil] * [g/10^6 ug] * density [g/m3] * depth [m]* A [m2]
# Soil bulk density: 2200 or 0.99? -> Leaching experiments: 0.99 [g/cm3]
rho = 0.99*10^6 # soil density [g/m3]
depth = 0.005 # [m]

# Transect Areas pre-corn applications
Area_Na = 13.92663*10^4 # [m2]
Area_Ta = 6.55813*10^4  # [m2]
Area_Sa = 11.05376*10^4 # [m2]

# Transect Areas post Corn applications
Area_Nb = 14.9949*10^4 # [m2]
Area_Tb = 6.55813*10^4  # [m2]
Area_Sb = 11.65202*10^4 # [m2]

# Assign new column for S-metolachlor mass in grams
comp.CoIs$MassSoil.g <- NA

# Areas with S-metolachlor before week 9
comp.CoIs$MassSoil.g <-
  ifelse((comp.CoIs$Transect == "N" & comp.CoIs$Wnum < 9),
         comp.CoIs$Conc.mug.g.dry.soil*10^-6*rho*depth*Area_Na,
  ifelse((comp.CoIs$Transect == "T" & comp.CoIs$Wnum < 9),
```

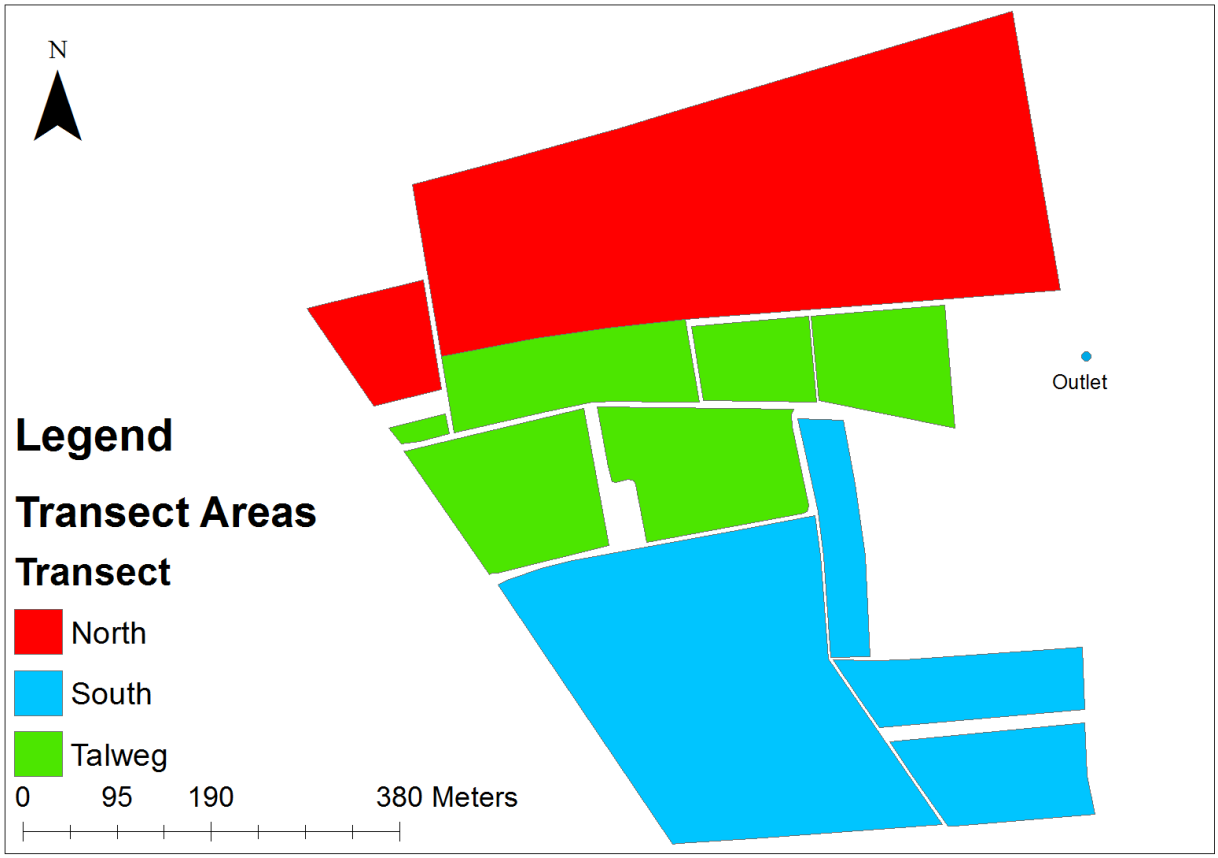

Figure 1: Transect Areas $[Ha]$ (North: 14.995; Talweg: 8.774; South: 12.668)

```
        comp.CoIs$Conc.mug.g.dry.soil*10^-6*rho*depth*Area_Ta,
  ifelse((comp.CoIs$Transect == "S" & comp.CoIs$Wnum < 9),
        comp.CoIs$Conc.mug.g.dry.soil*10^-6*rho*depth*Area_Sa, comp.CoIs$MassSoil.g)))

# Areas with S-metolachlor after week 9
comp.CoIs$MassSoil.g <-
  ifelse((comp.CoIs$Transect == "N" & comp.CoIs$Wnum >= 9),
        comp.CoIs$Conc.mug.g.dry.soil*10^-6*rho*depth*Area_Nb,
  ifelse((comp.CoIs$Transect == "T" & comp.CoIs$Wnum >= 9),
        comp.CoIs$Conc.mug.g.dry.soil*10^-6*rho*depth*Area_Tb,
  ifelse((comp.CoIs$Transect == "S" & comp.CoIs$Wnum >= 9),
        comp.CoIs$Conc.mug.g.dry.soil*10^-6*rho*depth*Area_Sb, comp.CoIs$MassSoil.g)))

print("S-meto mass per transect at time-t")
```

```
## [1] "S-meto mass per transect at time-t"
```

```
str(comp.CoIs)
```

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

Save files

```
write.csv2(comp.CoIs,
           'Data/WeeklySoils_Rng.csv', row.names = F)
```