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 at the end of the season is shown below. Corn fields in the catchment were known to have received S-metolachlor applications only during the last week of May, 2017. Given that two of these plots were not included within the transects, their area were not accounted for but until after the known application dates for corn plots.

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]

# Corrections (old values):
#Area_Ta = 6.55813*10^4  # [m2] # South Burger's as Talweg
#Area_Sa = 11.05376*10^4 # [m2] # South Burger's as Talweg
Area_Ta = 4.37134*10^4  # [m2]
Area_Sa = 13.3175*10^4 # [m2] # South Burger's as South

# Transect Areas post Corn applications (not on transect)
Area_Nb = 14.9949*10^4 # [m2]

# Corrections (old values):
#Area_Tb = 6.55813*10^4  # [m2] # South Burger's as Talweg
#Area_Sb = 11.65202*10^4 # [m2] # South Burger's as Talweg
```

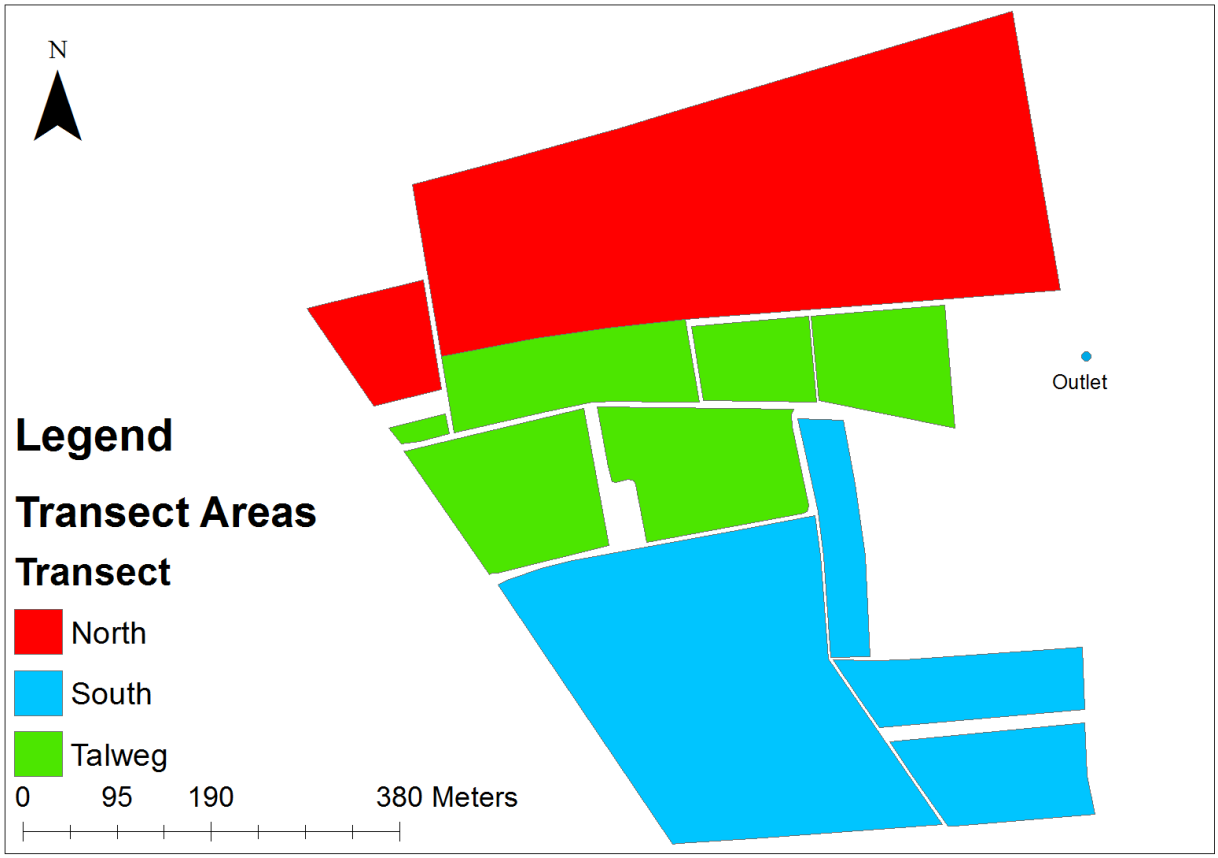

Figure 1: Transect Areas $[Ha]$ (North: 14.995; Talweg: 8.774; South: 12.668)

```
Area_Tb = 4.37134*10^4  # [m2]
Area_Sb = 13.91767*10^4 # [m2] # South Burger's as South




# 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),
         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)))

# Areas as variables (for later computation of bulk catchment mass)
comp.CoIs$Area.N <-
  ifelse((comp.CoIs$Wnum < 9), Area_Na, Area_Nb)

comp.CoIs$Area.T <-
  ifelse((comp.CoIs$Wnum < 9), Area_Ta, Area_Tb)

comp.CoIs$Area.S <-
  ifelse((comp.CoIs$Wnum < 9), Area_Sa, Area_Sb)


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  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               : 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 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 ...
```

```
tail(comp.CoIs)
```

```
##         ID Transect Wnum        Date.Soil             Date.ti
## 8  AW-N-14        N   14 04/07/2016 14:42 2016-07-04 14:42:00
## 25 AW-S-14        S   14 04/07/2016 14:42 2016-07-04 14:42:00
## 42 AW-T-14        T   14 04/07/2016 14:42 2016-07-04 14:42:00
## 9  AW-N-15        N   15 12/07/2016 01:00 2016-07-12 01:00:00
## 26 AW-S-15        S   15 12/07/2016 01:00 2016-07-12 01:00:00
## 43 AW-T-15        T   15 12/07/2016 01:00 2016-07-12 01:00:00
##    Conc.mug.g.dry.soil Conc.ComSoil.SD N_compsoil comp.d13C comp.d13C.SD
## 8            1.3336411      0.06825606          3 -27.16533    1.3381466
## 25           1.0220275      0.06825606          3 -27.83867    0.9586315
## 42           1.5868495      0.06825606          3 -26.08233    1.3480372
## 9            0.9564201      0.06825606         NA        NA           NA
## 26           1.1610022      0.06825606         NA        NA           NA
## 43           1.3119054      0.06825606         NA        NA           NA
##    comp.d13C.SE DD13C.comp     f.comp   B.comp f.min.comp B.min.comp
## 8     0.7725793   4.049067 0.06200468 93.79953 0.12425628   87.57437
## 25    0.5534661   3.375733 0.09837564 90.16244 0.17565709   82.43429
## 42    0.7782896   5.132067 0.02953162 97.04684 0.07123861   92.87614
## 9            NA         NA         NA       NA         NA         NA
## 26           NA         NA         NA       NA         NA         NA
## 43           NA         NA         NA       NA         NA         NA
##    f.mean.comp B.mean.com MassSoil.g Area.N  Area.T   Area.S
## 8   0.09224339   90.77566   989.8919 149949 43713.4 139176.7
## 25  0.13701268   86.29873   704.0999 149949 43713.4 139176.7
## 42  0.04884473   95.11553   343.3646 149949 43713.4 139176.7
## 9           NA         NA   709.9004 149949 43713.4 139176.7
## 26          NA         NA   799.8430 149949 43713.4 139176.7
## 43          NA         NA   283.8718 149949 43713.4 139176.7
```

Save files

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