

Mass Soils - Composite Weeks Alteck 2016

PAZ

November 2016

Purpose

This file merges weekly composite concentrations and isotope data.

Imports:

- SoilCompConc_W1toW15.csv
- SoilCompIsotopes_W1toW15.csv

Generates:

- WeeklySoils_Rng.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"
```

Lab Parameters

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

Field Assumptions

```
# S-metolachlor Mass [g]
# Conc. [ug/g dry soil] * [g/106 ug] * density [g/m3] * depth [m] * A [m2]
# Soil bulk density: 2200 or 0.99? -> Leaching experiments: 0.99 [g/cm3]
rho = 0.99*106 # soil density [g/m3]
depth = 0.01 # [m]

# Transect Areas pre-corn applications
Area_Na = 13.92663*104 # [m2]
```

```

# Assumptions on Non-measured plots - Transect assignment:
#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]

# Assumptions on Non-measured plots - Transect assignment:
#Area_Tb = 6.55813*10^4 # [m2] # South Burger's as Talweg
#Area_Sb = 11.65202*10^4 # [m2] # South Burger's as Talweg
Area_Tb = 4.37134*10^4 # [m2]
Area_Sb = 13.91767*10^4 # [m2] # South Burger's as South

Area_tot <- Area_Nb + Area_Tb + Area_Sb
Area_tot

## [1] 332839.1

# Areas touching each transect (respective to)needed for Rayleigh initial concentrations)
#Area_Nt <- 101721.702 # [m2]
#Area_Tt <- 39247.330
#Area_St <- 94205.501

```

Composite Concentrations & Isotope Data - Alteckendorf 2016

1. Import CSV files

```

#weeklySoilConc = read.csv2("Data/SoilCompConc_W1toW15.csv", header = TRUE)
# Date format stopped working in CSV
# Convert in CSV via "=TEXT(CELL.ID, "dd/mm/yyyy hh:mm")" based on xls-file date

weeklySoilConc = read.csv2("Data/SoilCompConc_W1toW15.csv", header = TRUE, dec = ".")
if (length(weeklySoilConc) == 1){
  weeklySoilConc = read.csv("Data/SoilCompConc_W1toW15.csv", header = TRUE)
}
head(weeklySoilConc)

```

```

##  Filename ID Transect Wnum Sample.Date      Date.Soil
## 1  AW-N-Ox AW      N    -1  30/03/2016  25/03/2016  00:04
## 2  AW-T-Ox AW      T    -1  30/03/2016  25/03/2016  00:04
## 3  AW-S-Ox AW      S    -1  30/03/2016  25/03/2016  00:04
## 4  AW-N-O AW      N     0  30/03/2016  30/03/2016  12:18
## 5  AW-T-O AW      T     0  30/03/2016  30/03/2016  12:18
## 6  AW-S-O AW      S     0  30/03/2016  30/03/2016  12:18
##  Conc.mug.g.dry.soil Conc.ComSoil.SD
## 1      0.06859297      0.01028895
## 2      0.04380646      0.00657097
## 3      0.07602098      0.01140315
## 4      1.03755848      0.15563377
## 5      0.93422934      0.14013440
## 6      3.73797761      0.56069664

```

```

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)
names(weeklySoilConc)

## [1] "Filename"          "ID"                  "Transect"
## [4] "Wnum"               "Sample.Date"         "Date.Soil"
## [7] "Conc.mug.g.dry.soil" "Conc.ComSoil.SD"     "Date.ti"

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  0.0686 0.0438 0.076 1.0376 0.9342 ...
##  $ Conc.ComSoil.SD   : num  0.01029 0.00657 0.0114 0.15563 0.14013 ...

# After nanogram revision
weeklySoilIso = read.csv2("Data/SoilCompIsotopes_W1toW15.csv", header = TRUE, dec = ".")
if (length(weeklySoilIso) == 1){
  weeklySoilIso = read.csv("Data/SoilCompIsotopes_W1toW15.csv", header = T)
}
colnames(weeklySoilIso)

## [1] "Filename" "ID"          "Transect" "Num"          "Repl"          "d.13C.12C"

weeklySoilIso$ID <- NULL
weeklySoilIso <- weeklySoilIso[complete.cases(weeklySoilIso[, "d.13C.12C"]), ]
weeklySoilIso$DD13 <- weeklySoilIso$d.13C.12C - -32.253
colnames(weeklySoilIso)[colnames(weeklySoilIso) == "Filename"] <- "ID"

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

isoCompSummary = ddpby(weeklySoilIso, c("ID"), summarise,

```

```

        N_compsoil = length(d.13C.12C),
        comp.d13C = mean(d.13C.12C),
        comp.d13C.SD = sd(d.13C.12C),
        N_isoComp = length(d.13C.12C)
        # comp.d13C.SE = comp.d13C.SD / sqrt(N_compsoil),
        # N_ngC = length(ngC),
        # ngC.mean = mean(ngC),
        # ngC.SD = sd(ngC) #,
        # ngC.SE = ngC.SD/sqrt(N_ngC)
    )

isoCompSummary$prctError <- (isoCompSummary$comp.d13C.SD/isoCompSummary$comp.d13C)*-100
mean(!is.na(isoCompSummary$prctError))

## [1] 0.9714286
# sum(isoCompSummary$N_ngC == 2)/(sum(isoCompSummary$N_ngC == 2) + sum(isoCompSummary$N_ngC > 2))

print("Soil Composites - Isotopes All")

## [1] "Soil Composites - Isotopes All"
str(weeklySoilIso)

## 'data.frame': 98 obs. of 3 variables:
## $ ID : Factor w/ 41 levels "AW-N-1","AW-N-10",...: 1 1 1 2 2 2 3 3 4 6 ...
## $ d.13C.12C: num -31.9 -31.4 -30.9 -29.9 -29.6 ...
## $ DD13 : num 0.363 0.863 1.353 2.353 2.693 ...
print("Soil Composites - Isotopes Ave and St.Dev.")

## [1] "Soil Composites - Isotopes Ave and St.Dev."
str(isoCompSummary)

## 'data.frame': 35 obs. of 6 variables:
## $ ID : Factor w/ 41 levels "AW-N-1","AW-N-10",...: 1 2 3 4 5 6 7 8 9 10 ...
## $ N_compsoil : int 3 3 2 1 2 3 3 3 2 3 ...
## $ comp.d13C : num -31.4 -29.8 -29.5 -29.5 -29 ...
## $ comp.d13C.SD: num 0.495 0.1935 0.0636 NaN 0.4031 ...
## $ N_isoComp : int 3 3 2 1 2 3 3 3 2 3 ...
## $ prctError : num 1.577 0.65 0.216 NaN 1.392 ...

2. Merge lab concentrations and isotopes

comp.CoIs = merge(weeklySoilConc, isoCompSummary, by = "ID", all = T)
comp.CoIs$Wnum = as.numeric(comp.CoIs$Wnum)
comp.CoIs <- comp.CoIs[order(comp.CoIs$Wnum),]
comp.CoIs$DD13C.comp <- (comp.CoIs$comp.d13C - (d13Co))

comp.CoIs$comp.IMP.d13C <- comp.CoIs$comp.d13C
comp.CoIs$comp.IMP.d13C[is.na(comp.CoIs$comp.d13C)] <-
ave(comp.CoIs$comp.d13C,
    comp.CoIs$Wnum,
    FUN= function(x) mean(x, na.rm = T))[is.na(comp.CoIs$comp.d13C)]

```

```
# comp.CoIs$comp.d13C <- ifelse(is.na(comp.CoIs$comp.d13C), comp.CoIs$comp.IMP.d13C, comp.CoIs$comp.d13C)

print("Merged Soil Concentrations and Isotopes")

## [1] "Merged Soil Concentrations and Isotopes"
str(comp.CoIs)

## 'data.frame': 51 obs. of 14 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 0.0686 0.076 0.0438 1.0376 3.738 ...
## $ Conc.ComSoil.SD : num 0.01029 0.0114 0.00657 0.15563 0.5607 ...
## $ 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_isoComp : int NA NA NA NA NA NA 3 3 3 3 ...
## $ prctError : num NA NA NA NA NA ...
## $ DD13C.comp : num NA NA NA NA NA ...
## $ comp.IMP.d13C : num NaN NaN NaN NaN NaN ...
```

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

For non-measured plots, the soil concentration and isotope measured at the nearest 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 was not accounted for but until after the known application dates for corn plots.

```
# Check values:
Area_Nb/10000
```

```
## [1] 14.9949
```

```
Area_Tb/10000
```

```
## [1] 4.37134
```

```
Area_Sb/10000
```

```
## [1] 13.91767
```

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

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

```
# S-metolachlor Mass [g]
# Conc. [ug/g dry soil] * [g/106 ug] * density [g/m3] * depth [m] * A [m2]
# Soil bulk density: 2200 or 0.99? -> Leaching experiments: 0.99 [g/cm3]
rho # soil density [g/m3]
```

```
## [1] 990000
```

```
depth # [m]
```

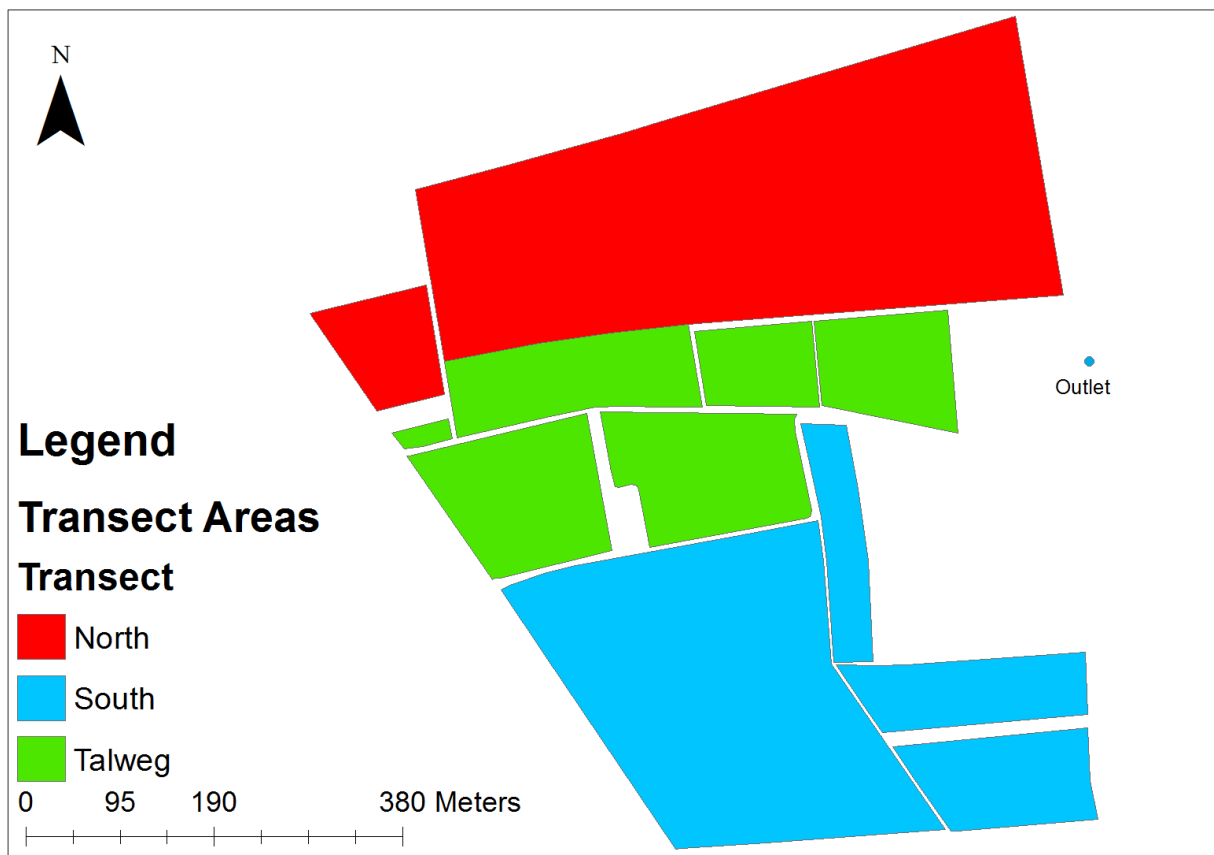


Figure 1: Transect Areas [Ha] (North: 14.995; Talweg: 4.371; South: 13.918)

```

## [1] 0.01
# Transect Areas pre-corn applications
Area_Na # [m2]

## [1] 139266.3
Area-Ta # [m2]

## [1] 43713.4
Area-Sa # [m2]

## [1] 133175
# Transect Areas post Corn applications (not on transect)
Area_Nb # [m2]

## [1] 149949
Area-Tb # [m2]

## [1] 43713.4
Area-Sb # [m2]

## [1] 139176.7
# Assign new column for S-metolachlor mass in grams
comp.CoIs$MassSoil.g <- NA
comp.CoIs$MassSoil.g.SD <- 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)))

comp.CoIs$MassSoil.g.SD <-
  ifelse((comp.CoIs$Transect == "N" & comp.CoIs$Wnum < 9),
    comp.CoIs$Conc.ComSoil.SD*10-6*rho*depth*Area_Na,
    ifelse((comp.CoIs$Transect == "T" & comp.CoIs$Wnum < 9),
      comp.CoIs$Conc.ComSoil.SD*10-6*rho*depth*Area-Ta,
      ifelse((comp.CoIs$Transect == "S" & comp.CoIs$Wnum < 9),
        comp.CoIs$Conc.ComSoil.SD*10-6*rho*depth*Area-Sa, comp.CoIs$MassSoil.g.SD)))

# 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)))

comp.CoIs$MassSoil.g.SD <-

```

```

ifelse((comp.CoIs$Transect == "N" & comp.CoIs$Wnum >= 9),
      comp.CoIs$Conc.ComSoil.SD*10-6*rho*depth*Area_Nb,
ifelse((comp.CoIs$Transect == "T" & comp.CoIs$Wnum >= 9),
      comp.CoIs$Conc.ComSoil.SD*10-6*rho*depth*Area_Tb,
ifelse((comp.CoIs$Transect == "S" & comp.CoIs$Wnum >= 9),
      comp.CoIs$Conc.ComSoil.SD*10-6*rho*depth*Area_Sb, comp.CoIs$MassSoil.g.SD)))

# 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)

# Needed to compute Transect res
#comp.CoIs$Area_Nt <- Area_Nt # [m2]
#comp.CoIs$Area_Tt <- Area_Tt
#comp.CoIs$Area_St <- Area_St

names(comp.CoIs)

## [1] "ID" "Transect" "Wnum"
## [4] "Date.Soil" "Date.ti" "Conc.mug.g.dry.soil"
## [7] "Conc.ComSoil.SD" "N_compsoil" "comp.d13C"
## [10] "comp.d13C.SD" "N_isoComp" "prctError"
## [13] "DD13C.comp" "comp.IMP.d13C" "MassSoil.g"
## [16] "MassSoil.g.SD" "Area.N" "Area.T"
## [19] "Area.S"

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 0.0686 0.076 0.0438 1.0376 3.738 ...
## $ Conc.ComSoil.SD : num 0.01029 0.0114 0.00657 0.15563 0.5607 ...
## $ 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_isoComp : int NA NA NA NA NA NA 3 3 3 3 ...
## $ prctError : num NA NA NA NA NA ...
## $ DD13C.comp : num NA NA NA NA NA ...
## $ comp.IMP.d13C : num NaN NaN NaN NaN NaN ...
## $ MassSoil.g : num 94.6 100.2 19 1430.5 4928.3 ...
## $ MassSoil.g.SD : num 14.19 15.03 2.84 214.58 739.24 ...

```



```
## $ 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      0.8163098      0.1224465      2      -28.965      0.4030509
## 25      1.1923654      0.1788548      NA      NA      NA
## 42      1.8513245      0.2776987      2      -27.900      0.1414214
## 9      1.1158234      0.1673735      NA      NA      NA
## 26      1.3545025      0.2031754      NA      NA      NA
## 43      1.5305563      0.2295834      NA      NA      NA
##      N_isoComp prctError DD13C.comp comp.IMP.d13C MassSoil.g MassSoil.g.SD
## 8      2 1.3915100      3.288      -28.9650 1211.8079      181.77118
## 25      NA      NA      NA      -28.4325 1642.8998      246.43497
## 42      2 0.5068866      4.353      -27.9000 801.1841      120.17761
## 9      NA      NA      NA      NaN 1656.4344      248.46516
## 26      NA      NA      NA      NaN 1866.3004      279.94506
## 43      NA      NA      NA      NaN 662.3676      99.35514
##      Area.N Area.T Area.S
## 8 149949 43713.4 139176.7
## 25 149949 43713.4 139176.7
## 42 149949 43713.4 139176.7
## 9 149949 43713.4 139176.7
## 26 149949 43713.4 139176.7
## 43 149949 43713.4 139176.7
```

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