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/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 = 0.01 # [m]

# Transect Areas pre-corn applications
Area_Na = 13.92663*10^4 # [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-0x AW        N   -1  30/03/2016 25/03/2016 00:04
## 2  AW-T-0x AW        T   -1  30/03/2016 25/03/2016 00:04
## 3  AW-S-0x AW        S   -1  30/03/2016 25/03/2016 00:04
## 4   AW-N-0 AW        N    0  30/03/2016 30/03/2016 12:18
## 5   AW-T-0 AW        T    0  30/03/2016 30/03/2016 12:18
## 6   AW-S-0 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 = ddply(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] 0.9705882
```

```
# 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':    96 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':    34 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.d13
```

```
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 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 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/10^6 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]
```
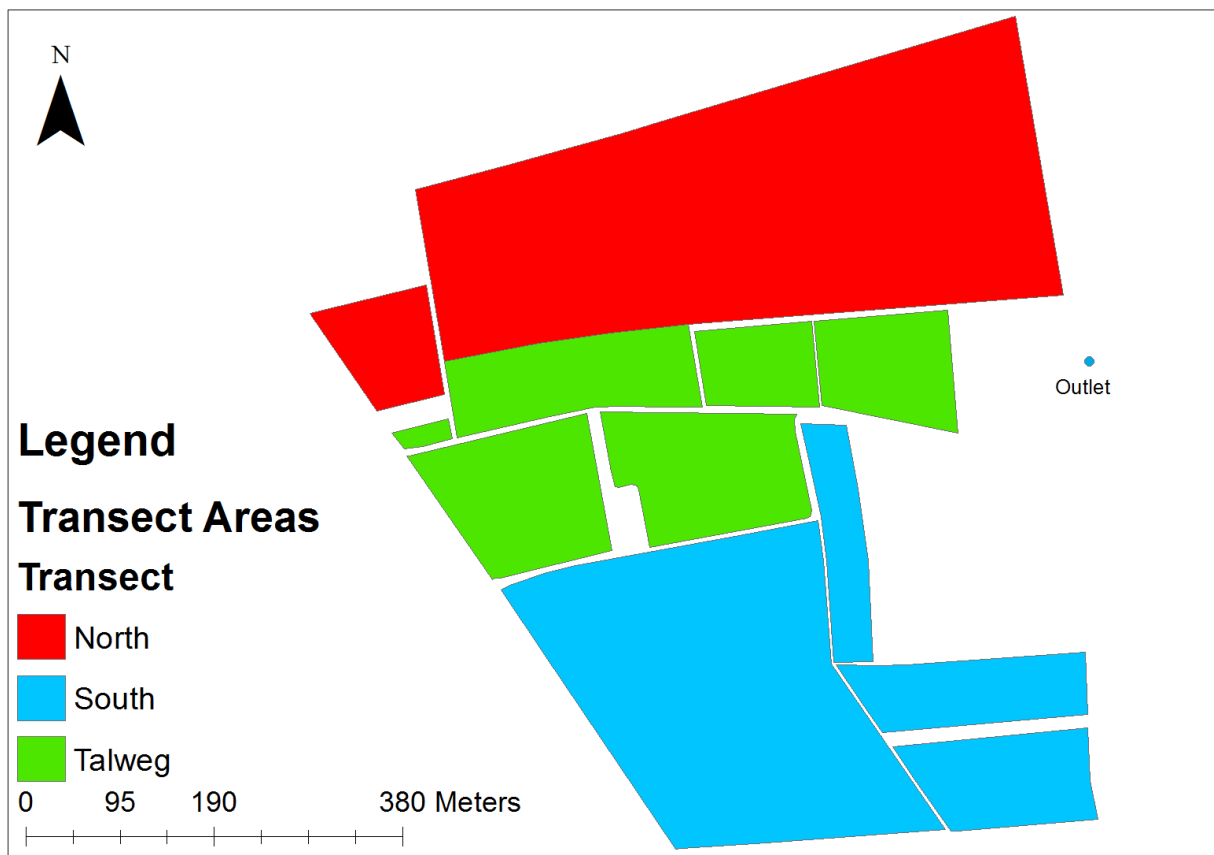
```
## [1] 990000
```

```
depth # [m]
```

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

```
## [1] 0.01
```

```r
# Transect Areas pre-corn applications
Area_Na # [m2]
```

```
## [1] 139266.3
```

```r
Area_Ta  # [m2]
```

```
## [1] 43713.4
```

```r
Area_Sa # [m2]
```

```
## [1] 133175
```

```r
# Transect Areas post Corn applications (not on transect)
Area_Nb # [m2]
```

```
## [1] 149949
```

```r
Area_Tb # [m2]
```

```
## [1] 43713.4
```

```r
Area_Sb # [m2]
```

```
## [1] 139176.7
```

```r
# 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 ...
```

```r
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            0.8117856       0.1017618          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  1205.0918     151.06492
## 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
```

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