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** (old, not used)
- **SoilCompIsotopes_W1toW15ng.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] "/Users/DayTightChunks/Documents/PhD/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           0.0180000              NA
## 2           0.0200000              NA
## 3           0.0290000              NA
## 4           0.8893358       0.1334004
## 5           0.8007680       0.1201152
## 6           3.2039808       0.4805971
```

```
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 0.889 0.801 ...
##  $ Conc.ComSoil.SD    : num  NA NA NA 0.133 0.12 ...
```

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

# After nanogram revision
weeklySoilIso  = read.csv2("Data/SoilCompIsotopes_W1toW15ng.csv", header = TRUE, dec = ".")
if (length(weeklySoilIso) == 1){
  weeklySoilIso = read.csv("Data/SoilCompIsotopes_W1toW15ng.csv", header = T)
}
head(weeklySoilIso)
```

```
##   Filename ID Week Num Repl d.13C.12C DD13.32.253. Ave...STDEV Deleted.d13
## 1   AW-N-1 AW    N   1    1 -31.88938        0.364       0.493
## 2   AW-N-1 AW    N   1    2 -31.39494        0.858
## 3   AW-N-1 AW    N   1    3 -30.90381        1.349                -29.546
## 4  AW-N-10 AW    N  10    1 -29.90000           NA
## 5  AW-N-10 AW    N  10    3 -29.56000           NA
## 6  AW-N-10 AW    N  10    4        NA           NA       0.197   -32.39275
##   Deleted.DD     Rt Ampl..44 Std.Ampl.   ng..C.
## 1            2648.2      120       904 3.982301
## 2            2648.0      115       904 3.816372
## 3      1.664 2648.0      109       904 3.617257
## 4            2655.6      155       658 7.066869
## 5            2656.4      183       658 8.343465
## 6      2.354     NA       NA        NA       NA
```

```r
colnames(weeklySoilIso)
```

```
##  [1] "Filename"     "ID"           "Week"         "Num"
##  [5] "Repl"         "d.13C.12C"    "DD13.32.253." "Ave...STDEV"
##  [9] "Deleted.d13"  "Deleted.DD"   "Rt"           "Ampl..44"
## [13] "Std.Ampl."    "ng..C."
```

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

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

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),
                       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
```

```r
sum(isoCompSummary$N_ngC == 2)/(sum(isoCompSummary$N_ngC == 2) + sum(isoCompSummary$N_ngC > 2))
```

```
## [1] 0.1764706
```

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

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

```r
str(weeklySoilIso)
```

```
## 'data.frame':    98 obs. of  4 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  0.364 0.858 1.349 2.353 2.693 ...
##  $ ngC      : num  3.98 3.82 3.62 7.07 8.34 ...
```

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

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

```r
str(isoCompSummary)
```

```
## 'data.frame':    35 obs. of  8 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  0.4928 0.1946 0.0636 NA 0.4031 ...
##  $ N_ngC       : int  3 3 2 1 2 3 3 3 2 3 ...
##  $ ngC.mean    : num  3.81 NA 8.64 1.57 5.12 ...
##  $ ngC.SD      : num  0.183 NA 0.806 NA 0.503 ...
##  $ prctError   : num  1.57 0.653 0.216 NA 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$comp.IMP.d13C <- comp.CoIs$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(c


# comp.CoIs$comp.d13C <- ifelse(is.na(comp.CoIs$comp.d13C), comp.CoIs$comp.IMP.d13C, comp.CoIs$comp.d13

comp.CoIs$DD13C.comp <- (comp.CoIs$comp.d13C - (d13Co))

print("Merged Soil Concentrations and Isotopes")
```

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

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

```
## 'data.frame':    51 obs. of  16 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 0.889 3.204 ...
##  $ Conc.ComSoil.SD    : num  NA NA NA 0.133 0.481 ...
##  $ 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_ngC              : int  NA NA NA NA NA NA 3 3 3 3 ...
##  $ ngC.mean           : num  NA NA NA NA NA ...
##  $ ngC.SD             : num  NA NA NA NA NA ...
##  $ prctError          : num  NA NA NA NA NA ...
##  $ comp.IMP.d13C      : num  NaN NaN NaN NaN NaN ...
##  $ DD13C.comp         : num  NA NA NA NA NA ...
```

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.

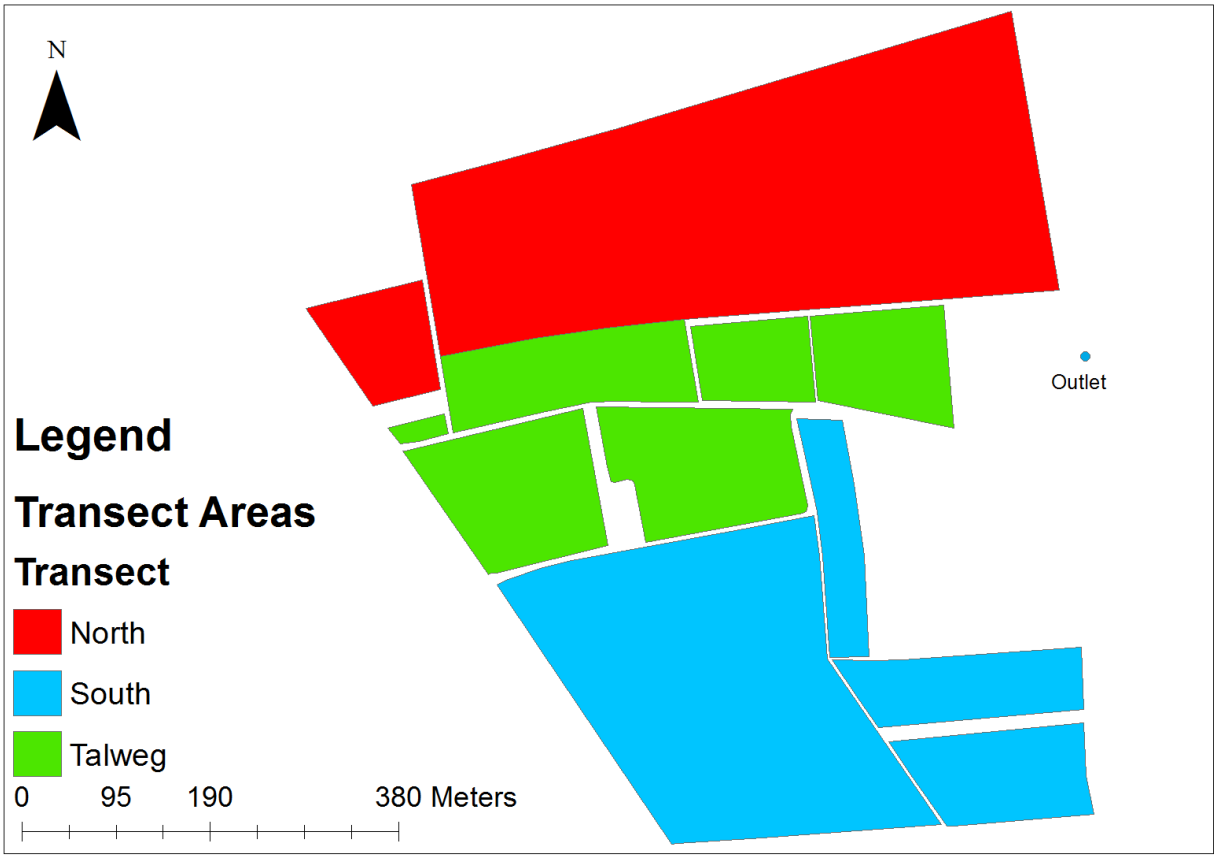

Figure 1: Transect Areas $[Ha]$ (North: 14.995; Talweg: 4.371; South: 13.918)

```
# 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]
```

```
## [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_ngC"             "ngC.mean"
## [13] "ngC.SD"            "prctError"         "comp.IMP.d13C"
## [16] "DD13C.comp"        "MassSoil.g"        "MassSoil.g.SD"
## [19] "Area.N"            "Area.T"            "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  21 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 0.889 3.204 ...
##  $ Conc.ComSoil.SD    : num  NA NA NA 0.133 0.481 ...
##  $ 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_ngC              : int  NA NA NA NA NA NA 3 3 3 3 ...
##  $ ngC.mean           : num  NA NA NA NA NA ...
##  $ ngC.SD             : num  NA NA NA NA NA ...
##  $ prctError          : num  NA NA NA NA NA ...
##  $ comp.IMP.d13C      : num  NaN NaN NaN NaN NaN ...
##  $ DD13C.comp         : num  NA NA NA NA NA ...
##  $ MassSoil.g         : num  24.82 38.23 8.66 1226.16 4224.23 ...
##  $ MassSoil.g.SD      : num  NA NA NA 184 634 ...
##  $ 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       0.2000462          2   -28.965    0.4030509
## 25           1.0220275       0.1533041         NA        NA           NA
## 42           1.5868495       0.2380274          2   -27.900    0.1414214
## 9            0.9564201       0.1434630         NA        NA           NA
## 26           1.1610022       0.1741503         NA        NA           NA
## 43           1.3119054       0.1967858         NA        NA           NA
##    N_ngC ngC.mean    ngC.SD prctError comp.IMP.d13C DD13C.comp MassSoil.g
## 8      2 5.118483 0.5026825 1.3915100      -28.9650      3.288  1979.7837
## 25    NA       NA        NA        NA      -28.4325         NA  1408.1998
## 42     2 5.699301 0.9395125 0.5068866      -27.9000      4.353   686.7292
## 9     NA       NA        NA        NA           NaN         NA  1419.8009
## 26    NA       NA        NA        NA           NaN         NA  1599.6860
## 43    NA       NA        NA        NA           NaN         NA   567.7437
##    MassSoil.g.SD Area.N  Area.T   Area.S
## 8      296.96756 149949 43713.4 139176.7
## 25     211.22998 149949 43713.4 139176.7
```

```
## 42     103.00938 149949 43713.4 139176.7
## 9      212.97013 149949 43713.4 139176.7
## 26     239.95291 149949 43713.4 139176.7
## 43      85.16155 149949 43713.4 139176.7
```

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