

Observed Data Prep for Model Analysis

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Purpose

Generate BEACH calibration data with:

- groupAlteck2016_R.csv (Book 04)

Lab parameters and field constants

```
if (MAC) {  
  if (WIN){  
    path = file.path("C:/Users/DayTimeChunks/Documents/PhD/HydrologicalMonitoring")  
  
  } else {  
    # path = file.path("/Users/DayTightChunks/Documents/PhD/HydrologicalMonitoring")  
    path = file.path("/Users/DayTightChunks/Documents/PhD/HydroMonitor/.nosync/HydrologicalMonitoring")  
  }  
} else {  
  path = file.path("D:/Documents/these_pablo/Alteckendorf2016/HydrologicalMonitoring")  
  time = read.csv2("D:/Documents/these_pablo/Models/BEACH2016/Analysis/Data/Time.csv")  
  time$DayMoYr = as.POSIXct(strptime(time$date, "%d/%m/%Y", tz="EST"))  
}  
source(file.path(path, "global.R"))
```

Packages

```
# Plotting functions  
library("scales")  
library("tidyverse")  
  
## Warning: package 'tidyverse' was built under R version 3.3.3  
library("dplyr")  
library("reshape")  
library("zoo") # na.approx()
```

Working directory

```
# setwd("D:/Documents/these_pablo/Alteckendorf2016/R")  
  
# MAC  
# setwd("/Users/DayTightChunks/Documents/PhD/Routput/Alteck/R")
```

```

# Mac-WIN
# setwd("C:/Users/DayTightChunks/Documents/Models/pesti-beach16/Analysis/Data")
getwd()

## [1] "D:/Documents/these_pablo/Models/BEACH2016/Analysis/Data"



## Discharge & Response Variables (with markers)



- Ignoring  $\delta$  in filters (for now)



```

q = read.csv2(file.path(path, "Data/groupAlteck2016_R.csv"))
q$Vol.L = q$Vol2min * 1000

q = q[, c("Date", "DateCheck", "Q.HW1", "DayMoYr", "Vol.L", "sampleQ", "Type", "SubWeeks", "Weeks", "W")]
names(q)

[1] "Date" "DateCheck" "Q.HW1" "DayMoYr" "Vol.L"
[6] "sampleQ" "Type" "SubWeeks" "Weeks" "WeekNo"

mark = read.csv(file.path(path, "Data/MarkerResponse_R05.csv"))
mark = mark[, c("WeekSubWeek",
 "# AveDischarge.m3.h", "Volume.m3", "Sampled.Hrs",
 "# Sampled",
 "Conc.mug.L", "Conc.SD",
 "# Vol.SPE.L", "Conc.in500uL",
 "OXA_mean", "OXA_SD", "ESA_mean", "ESA_SD",
 "N.x", "diss.d13C", "SD.d13C",
 "MES.mg.L", "MES.sd", "MO.mg.L", "Conc.Solids.mug.gMES", "Conc.Solids.ug.gMES.SD" #,
 "#N.y", "filt.d13C", "filt.SD.d13C" #,
 "#DD13C.diss", "DD13C.filt"
)]
names(mark)

[1] "WeekSubWeek" "Conc.mug.L"
[3] "Conc.SD" "OXA_mean"
[5] "OXA_SD" "ESA_mean"
[7] "ESA_SD" "N.x"
[9] "diss.d13C" "SD.d13C"
[11] "MES.mg.L" "MES.sd"
[13] "MO.mg.L" "Conc.Solids.mug.gMES"
[15] "Conc.Solids.ug.gMES.SD"

Delete repeated W6 observation, or with NA in week markers
mark = mark[mark$WeekSubWeek != as.character("W6-3j7") & !is.na(mark$WeekSubWeek),]

```



```

q$Date = as.POSIXct(strptime(q$DateCheck, "%d/%m/%Y %H:%M", tz="EST"))
q$DayMoYr = as.POSIXct(strptime(q$DateCheck, "%d/%m/%Y", tz="EST"))
q$Min = 2.0

CHECK0 = F
if (CHECK0){
 sum(is.na(q$Date))

```


```

```

naDates = q[is.na(q$Date == TRUE),]

duplicateAlteck <- q[duplicated(q$DateCheck),]
head(duplicateAlteck)
}

```

Prepare Volume Discharged Time Series (TSS)

```

qDay <- q %>%
  group_by(DayMoYr) %>%
  dplyr::summarize(Volday.L = sum(Vol.L))

qDay$VolTot.m3 = round(qDay$Volday.L/10^3, 3)

qTime = merge(time, qDay, by = "DayMoYr", all = T)

mean(qTime$VolTot.m3, na.rm = T)

## [1] 259.9841
sd(qTime$VolTot.m3, na.rm = T)

## [1] 453.5581

Volm3_tss = qTime[,c("Jdays", "VolTot.m3")]

Volm3_tss$VolTot.m3 = ifelse(is.na(Volm3_tss$VolTot.m3), -1.0, Volm3_tss$VolTot.m3)

if (F) {
  write.table(Volm3_tss, "BEACH_R/q_obs_m3day.tss", sep="\t", row.names = F, col.names = F)
}

if (F) {

  ## Convert m3.h -> m3
  qDay <- q %>%
    group_by(DayMoYr) %>%
    dplyr::summarize(Q.m3 = sum(Vol2min))

  qDay$Q.mm = (qDay$Q.m3/catchment_area)*10^3

  qDay$time = seq.int(nrow(qDay))

  # Qm3/day
  DischQm3_tss = qDay[,c("time", "Q.m3")]
  write.table(DischQm3_tss, "BEACH_R/disch_m3day.tss", sep="\t", row.names = F, col.names = F)

  # Qmm/day
  DischQmm_tss = qDay[,c("time", "Q.mm")]
  write.table(DischQmm_tss, "BEACH_R/disch_mmday.tss", sep="\t", row.names = F)
}

```

Merge 2-min disch with sub-weekly markers

- Convert to mass (and corresponding SD) discharged

```
qm = merge(q, mark, by.x = "SubWeeks", by.y = "WeekSubWeek", all = T)

# Dissolved
qm$SmetOut_ug.obs = qm$Vol.L*qm$Conc.mug.L
qm$SmetOut_ug.sd = qm$Vol.L*qm$Conc.SD
qm$OxaOut_ug.obs = qm$Vol.L*qm$OXA_mean
qm$OxaOut_ug.sd = qm$Vol.L*qm$OXA_SD
qm$EsaOut_ug.obs = qm$Vol.L*qm$ESA_mean
qm$EsaOut_ug.sd = qm$Vol.L*qm$ESA_SD

# Suspended Solids (SS)
# Smet.ug in SS = ug/g * (MES [mg/L] * [1g/10^3mg]) * Vol [L]
qm$SmetSS_ug.obs = qm$Conc.Solids.mug.gMES * (qm$MES.mg.L*10^-3) * qm$Vol.L
qm$SmetSS_ug.sd = qm$Conc.Solids.ug.gMES.SD * (qm$MES.sd*10^-3) * qm$Vol.L

qm$MassDelta.obs = qm$SmetOut_ug.obs*qm$diss.d13C
qm$MassDelta.sd = qm$SmetOut_ug.sd*qm$SD.d13C

names(qm)

## [1] "SubWeeks"                  "Date"
## [3] "DateCheck"                 "Q.HW1"
## [5] "DayMoYr"                   "Vol.L"
## [7] "sampleQ"                   "Type"
## [9] "Weeks"                      "WeekNo"
## [11] "Min"                        "Conc.mug.L"
## [13] "Conc.SD"                    "OXA_mean"
## [15] "OXA_SD"                     "ESA_mean"
## [17] "ESA_SD"                     "N.x"
## [19] "diss.d13C"                 "SD.d13C"
## [21] "MES.mg.L"                  "MES.sd"
## [23] "M0.mg.L"                   "Conc.Solids.mug.gMES"
## [25] "Conc.Solids.ug.gMES.SD"   "SmetOut_ug.obs"
## [27] "SmetOut_ug.sd"              "OxaOut_ug.obs"
## [29] "OxaOut_ug.sd"              "EsaOut_ug.obs"
## [31] "EsaOut_ug.sd"              "SmetSS_ug.obs"
## [33] "SmetSS_ug.sd"              "MassDelta.obs"
## [35] "MassDelta.sd"
```

Compute by-day & by-subweek

- ignoring solids (for now)

We need to obtain a bulk concentration for the day, not by taking the mean concentration, but rather the proportional mass contribution of each sub-sample, determined by the relative volume such that the concentration of each daily sample (C_i) is :

$$C_{bulksample} = \frac{C_1 \cdot V_1 + C_2 \cdot V_2}{V_{tot}} \quad (1)$$

To obtain the bulk concentration (and because there are overlaps of some days across subsamples) we need to first to:

1. Convert discharge mass to concentration
2. Interpolate concentrations (and deltas) of only the duplicate days, where no sample was possible

```
# Step 1
# Sum masses by day, without mixing days from different samples (the latter will be 'duplicate' days)
qmDay <- qm %>%
  group_by(DayMoYr, SubWeeks) %>%
  dplyr::summarize(Volday.L = sum(Vol.L),
                   SmpHrs = sum(Min)/60,
                   SmOut_ug.obs = sum(SmetOut_ug.obs),
                   SmOut_ug.sd = (sum(SmetOut_ug.sd^2))^0.5, # Cumulative SD
                   OxOut_ug.obs = sum(OxaOut_ug.obs),
                   OxOut_ug.sd = (sum(OxaOut_ug.sd^2))^0.5, # Cumulative SD
                   EsOut_ug.obs = sum(EsaOut_ug.obs),
                   EsOut_ug.sd = (sum(EsaOut_ug.sd^2))^0.5, # Cumulative SD
                   ConcSmOut_ugL.obs = SmOut_ug.obs/Volday.L, # Smet
                   ConcSmOut_ugL.sd = SmOut_ug.sd/Volday.L,
                   ConcOxOut_ugL.obs = OxOut_ug.obs/Volday.L, # Oxa
                   ConcOxOut_ugL.sd = OxOut_ug.sd/Volday.L,
                   ConcEsOut_ugL.obs = EsOut_ug.obs/Volday.L, # Esa
                   ConcEsOut_ugL.sd = EsOut_ug.sd/Volday.L,
                   delta.obs = sum(MassDelta.obs)/(sum(SmetOut_ug.obs)),
                   delta.sd = (sum(MassDelta.sd^2))^0.5/(sum(SmetOut_ug.sd^2))^0.5
  )

# Step 2
# Get all duplicated days with data
allDup = qmDay %>%
  group_by(DayMoYr) %>%
  filter(n()>1 & !is.na(SmOut_ug.obs))

# Do flow proportional average
qmBlkDup = allDup %>%
  group_by(DayMoYr) %>%
  dplyr::summarize(VolTot.L = sum(Volday.L),
                   TotHrs = sum(SmpHrs),
                   ConSmOut_ugL.blk = sum(ConcSmOut_ugL.obs * Volday.L)/sum(Volday.L),
                   ConSmOut_ugL.sd = sum(ConcSmOut_ugL.sd * Volday.L)/sum(Volday.L),
                   ConOxOut_ugL.blk = sum(ConcOxOut_ugL.obs * Volday.L)/sum(Volday.L),
                   ConOxOut_ugL.sd = sum(ConcOxOut_ugL.sd * Volday.L)/sum(Volday.L),
                   ConEsOut_ugL.blk = sum(ConcEsOut_ugL.obs * Volday.L)/sum(Volday.L),
                   ConEsOut_ugL.sd = sum(ConcEsOut_ugL.sd * Volday.L)/sum(Volday.L),
                   deltaOut.blk = sum(delta.obs * Volday.L)/sum(Volday.L),
                   deltaOut.sd = sum(delta.sd * Volday.L)/sum(Volday.L)
  )

# Removed rows - Only for reference (not used)
removed = qmDay %>%
  group_by(DayMoYr) %>%
  filter(n()>1 & is.na(SmOut_ug.obs))

removedBlk = removed %>%
```

```

group_by(DayMoYr) %>%
dplyr::summarize(VolTot.L = sum(Volday.L),
                  TotHrs = sum(SmpHrs),
                  ConSmOut_ugL.blk = sum(ConcSmOut_ugL.obs * Volday.L)/sum(Volday.L),
                  ConSmOut_ugL.sd = sum(ConcSmOut_ugL.sd * Volday.L)/sum(Volday.L),
                  ConOxOut_ugL.blk = sum(ConcOxOut_ugL.obs * Volday.L)/sum(Volday.L),
                  ConOxOut_ugL.sd = sum(ConcOxOut_ugL.sd * Volday.L)/sum(Volday.L),
                  ConEsOut_ugL.blk = sum(ConcEsOut_ugL.obs * Volday.L)/sum(Volday.L),
                  ConEsOut_ugL.sd = sum(ConcEsOut_ugL.sd * Volday.L)/sum(Volday.L),
                  deltaOut.blk = sum(delta.obs * Volday.L)/sum(Volday.L),
                  deltaOut.sd = sum(delta.sd * Volday.L)/sum(Volday.L)
                )

# Get all non-duplicated days. do average to get same variables
ndup = qmDay %>%
  group_by(DayMoYr) %>%
  filter(n()==1)

qmBlk_nDup = ndup %>%
  group_by(DayMoYr) %>%
  dplyr::summarize(VolTot.L = sum(Volday.L),
                  TotHrs = sum(SmpHrs),
                  ConSmOut_ugL.blk = sum(ConcSmOut_ugL.obs * Volday.L)/sum(Volday.L),
                  ConSmOut_ugL.sd = sum(ConcSmOut_ugL.sd * Volday.L)/sum(Volday.L),
                  ConOxOut_ugL.blk = sum(ConcOxOut_ugL.obs * Volday.L)/sum(Volday.L),
                  ConOxOut_ugL.sd = sum(ConcOxOut_ugL.sd * Volday.L)/sum(Volday.L),
                  ConEsOut_ugL.blk = sum(ConcEsOut_ugL.obs * Volday.L)/sum(Volday.L),
                  ConEsOut_ugL.sd = sum(ConcEsOut_ugL.sd * Volday.L)/sum(Volday.L),
                  deltaOut.blk = sum(delta.obs * Volday.L)/sum(Volday.L),
                  deltaOut.sd = sum(delta.sd * Volday.L)/sum(Volday.L)
                )

# Bind Bulk samples
qmBlk = rbind(qmBlkDup, qmBlk_nDup)

qmBlk90 = qmBlk %>%
  filter(TotHrs >= 21.6)

qmBlk50 = qmBlk %>%
  filter(TotHrs >= 12.0)

# Get dates/markers column
m <- q %>%
  group_by(DayMoYr) %>%
  dplyr::summarise(SubWeeks = SubWeeks[1])

qmBlk90_obs = merge(qmBlk90, m, by = "DayMoYr", all = T)
qmBlk50_obs = merge(qmBlk50, m, by = "DayMoYr", all = T)

qmBlk90_obs = qmBlk90_obs[order(qmBlk90_obs$DayMoYr), ]
qmBlk50_obs = qmBlk50_obs[order(qmBlk50_obs$DayMoYr), ]

```

```

# Natural log (ln) for low concentrations
qmBlk90$lnConSmOut_ugL.blk = log(qmBlk90$ConSmOut_ugL.blk)

mean(qmBlk90$ConSmOut_ugL.blk, na.rm = T) # = 1.9897
## [1] 1.989693
mean(qmBlk90$lnConSmOut_ugL.blk, na.rm = T) # -0.644
## [1] -0.644245
mean(qmBlk90$deltaOut.blk, na.rm = T) # -30.52
## [1] -30.519

```

3. Obtain approximate total mass discharged (without interpolation)

```

qmBlk_mass = merge(qmBlk, m, by = "DayMoYr", all = T)
# Interpolate bulk concentrations to obtain a cumulative mass discharged
# Att:!!! not to use concentration as observation point, only as approximate loading totals
# Convert to grams (to match model output)
qmBlk_mass$MassSmOut_g = ((qmBlk_mass$ConSmOut_ugL.blk)/10**6)*qmBlk_mass$VolTot.L
qmBlk_mass$MassSmOut_g = ifelse(is.na(qmBlk_mass$MassSmOut_g), 0, qmBlk_mass$MassSmOut_g)
qmBlk_mass$CumMassSmOut_g = cumsum(qmBlk_mass$MassSmOut_g)

```

4. Incorporate Julian days before saving

```

qmBlk90 = merge(time, qmBlk90, by = "DayMoYr", all = T)
qmBlk_mass = merge(time, qmBlk_mass, by = "DayMoYr", all = T)

if (F) {
  # write.csv(qmBlk, "qmBlk_R.csv", row.names = F) # , sep = ";", dec = ".")
}

```

Get S-met Concentrations ($\geq 90\%$ of day samples) AND Mass export Time Series (TSS)

```

Conc_ugL_tss = qmBlk90[,c("Jdays", "ConSmOut_ugL.blk")]
Conc_ugL_tss$ConSmOut_ugL.blk = ifelse(is.na(Conc_ugL_tss$ConSmOut_ugL.blk), -1e9, Conc_ugL_tss$ConSmOut_ugL.blk)

Mass_g_tss = qmBlk_mass[,c("Jdays", "MassSmOut_g")]
Mass_g_tss$MassSmOut_g = ifelse(is.na(Mass_g_tss$MassSmOut_g), -1e9, Mass_g_tss$MassSmOut_g)

CumMass_g_tss = qmBlk_mass[,c("Jdays", "CumMassSmOut_g")]
CumMass_g_tss$CumMassSmOut_g = ifelse(is.na(CumMass_g_tss$CumMassSmOut_g), -1e9, CumMass_g_tss$CumMassSmOut_g)

```

Get $\delta^{13}C$ time series (TSS)

```

Delta_out_tss = qmBlk90[,c("Jdays", "deltaOut.blk")]
Delta_out_tss$deltaOut.blk = ifelse(is.na(Delta_out_tss$deltaOut.blk), 1e9, Delta_out_tss$deltaOut.blk)

```

Save time series

```
if (F){  
  write.table(Conc_ugL_tss, "BEACH_R/Conc_ugL.tss", sep="\t", row.names = F, col.names = F)  
  write.table(Delta_out_tss, "BEACH_R/Delta_out.tss", sep="\t", row.names = F, col.names = F)  
}  
  
if (F){  
  write.table(Mass_g_tss, "BEACH_R/MassOut_g.tss", sep="\t", row.names = F, col.names = F)  
  write.table(CumMass_g_tss, "BEACH_R/CumMass_g.tss", sep="\t", row.names = F, col.names = F)  
}
```

Analyse Discharge Monthly Values

```
if (F) {  
  qDay$Month <-  
    ifelse(qDay$DayMoYr >= as.POSIXct("2016-03-24 00:30:00", tz = "EST") &  
           qDay$DayMoYr < as.POSIXct("2016-04-01 00:00:00", tz = "EST"), "March",  
    ifelse(qDay$DayMoYr >= as.POSIXct("2016-04-01 00:00:00", tz = "EST") &  
           qDay$DayMoYr < as.POSIXct("2016-05-01 00:00:00", tz = "EST"), "April",  
    ifelse(qDay$DayMoYr >= as.POSIXct("2016-05-01 00:00:00", tz = "EST") &  
           qDay$DayMoYr < as.POSIXct("2016-06-01 00:00:00", tz = "EST"), "May",  
    ifelse(qDay$DayMoYr >= as.POSIXct("2016-06-01 00:00:00", tz = "EST") &  
           qDay$DayMoYr < as.POSIXct("2016-07-01 00:00:00", tz = "EST"), "June",  
    )  
  )  
  
  dischSumm <- qDay %>%  
    group_by(Month) %>%  
    dplyr::summarize(MeanQmm = mean(Q.mm),  
                     SdevQmm = sd(Q.mm),  
                     MeanQm3 = mean(Q.m3))  
}
```