Carbonate Chemistry

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Installing older seacarb package and OTools package

Uncomment lines 13 and 14 if you need to install those packages.

Calculating pH from spectrophotometric data

Getting file names

```
files=list.files(recursive=T)
```

Selecting only the pH data

```
files.ph=files[grep("Spec_pH_Data",files)]
```

Running the first dataset

First we extract the date form the filename.

```
date.ph=gsub(".*(\\d\\d)_(\\d\\d)_(\\d\\d).ods","\\1-\\2-\\3",files.ph[1])
```

Then read in the dataset.

```
data.ph=read_ods(files.ph[1],col_names=T)
```

Now, we calculated the pH of all measurements in the file with the specpH() function.

```
ph=specpH(data.ph$S,data.ph$T,data.ph$A434,data.ph$A578,data.ph$A730,data.ph$B434,
          data.ph$B578,data.ph$B730)
```

Next, we gets the mean pH calculated for each tank.

```
ph.means=aggregate(ph~data.ph$Tank,FUN="mean")
```

Finally, do some formatting.

```
colnames(ph.means)[1]="tank"
ph.means$date=date.ph
ph.means$S=aggregate(data.ph$S~data.ph$Tank,FUN="mean")[,2]
carbchem=ph.means
```

Repeating the process with each of the following datasets and adding them to he dataset.

```
for (i in 2:length(files.ph)){
  date.ph=gsub(".*(\\d\\d)_(\\d\\d)_(\\d\\d).ods","\\1-\\2-\\3",files.ph[i])
  data.ph=read_ods(files.ph[i],col_names=T)
```

```
  ph=specpH(data.ph$S,data.ph$T,data.ph$A434,data.ph$A578,data.ph$A730,
            data.ph$B434,data.ph$B578,data.ph$B730)
  ph.means=aggregate(ph~data.ph[,1],FUN="mean")
  colnames(ph.means)[1]="tank"
  ph.means$date=date.ph
  ph.means$S=aggregate(data.ph[,3]~data.ph[,1],FUN="mean")[,2]

  carbchem=rbind(carbchem,ph.means)
}
```

Calculating alkalinity from titration data

Similar to how we did with the pH data, we extract the tank # from the filename, then read in the data and calculate the alkalinity from the data. Finally, we will organize it into a dataframe called "alk".

```
files.ti=files[grep("Titration_data/Titration",files)]

ti.tank=gsub(".*Tank (\\d+) Run \\d.ods","\\1",files.ti[1])
ti.filename=gsub(".*Titration_data/(.*)\\.ods","\\1",files.ti[1])
ti=read_ods(files.ti[1],col_names = T)
ti.at=at(ti[1,1],ti[1,8],ti[1,2],1,ti[1,3],ti[1,4],ti[1,5],ti[,6],ti[,7])[1]
alk=data.frame(filename=ti.filename,tank=ti.tank,alk=ti.at)
```

Then, we repeat for the rest of the data in the folder.

```
for (i in 2:length(files.ti)){
  ti.tank=gsub(".*Tank (\\d+) Run \\d.ods","\\1",files.ti[i])
  ti.filename=gsub(".*Titration_data/(.*)\\.ods","\\1",files.ti[i])
  ti=read_ods(files.ti[i],col_names = T)
  ti.at=at(ti[1,1],ti[1,8],ti[1,2],1,ti[1,3],ti[1,4],ti[1,5],ti[,6],ti[,7])[1]
  alk=rbind(alk,data.frame(filename=ti.filename,tank=ti.tank,alk=ti.at))
}
```

Now, we get the alkalinity mean for each tank.

```
alk.means=aggregate(alk~tank,data=alk,FUN="mean")
```

We take the mean alkalniity for each tank and put it into the carbchem dataset with the pH values.

```
carbchem=carbchem[carbchem$tank %in% alk.means$tank,]
carbchem$alk=0

for (i in 1:nrow(carbchem)){
  carbchem$alk[i]=alk.means$alk[alk.means$tank==carbchem$tank[i]]
}
```

Calculating pCO2 from the data

```
carbchem$pco2=carb(8,carbchem$ph,carbchem$alk,carbchem$S,10.8)$pCO2
```

Writing the data out to a .cvs file

```
write.csv(carbchem,"carbonate_chemistry.csv",row.names = F)
```

The final dataset

```
carbchem
```

```
##    tank         ph     date       S           alk        pco2
## 1     2 7.63841845 05-08-20 31.1000 0.00206197991 1023.888293
## 2     3 7.67879023 05-08-20 30.9000 0.00207103545  932.962916
## 5     6 7.63799829 05-08-20 31.1000 0.00205107662 1019.452077
## 7     8 7.62880241 05-08-20 30.9000 0.00209886552 1068.448970
## 8     9 7.79383014 05-08-20 30.6000 0.00206630891  702.050711
## 9    10 7.89748802 05-08-20 31.2000 0.00205467181  535.614019
## 10   11 7.92609874 05-08-20 31.0000 0.00200576246  486.601901
## 11    2 7.66779271 06-08-20 30.6000 0.00206197991  956.015404
## 12    3 7.64627996 06-08-20 31.1000 0.00207103545 1008.902324
## 15    6 7.62610290 06-08-20 31.4000 0.00205107662 1047.554257
## 17    8 7.62251466 06-08-20 31.1000 0.00209886552 1083.604468
## 18    9 7.64997162 06-08-20 30.9000 0.00206630891  998.777712
## 19   10 7.62741240 06-08-20 31.6000 0.00205467181 1044.844491
## 20   11 7.62250140 06-08-20 31.5000 0.00200576246 1032.548807
## 21    2 7.49224396 09-08-20 30.7000 0.00206197991 1461.591989
## 22    3 7.71995034 09-08-20 31.1000 0.00207103545  842.138189
## 23    8 7.52124824 09-08-20 30.7000 0.00209886552 1387.778304
## 24    9 7.74170984 09-08-20 31.0000 0.00206630891  796.772541
## 25   10 7.52611476 09-08-20 30.9000 0.00205467181 1340.889798
## 26   11 7.84381951 09-08-20 31.6000 0.00200576246  596.843530
## 27    2 7.44717922 10-08-20 30.3000 0.00206197991 1632.023695
## 28    3 7.74546303 10-08-20 30.7000 0.00207103545  792.834149
## 29    8 7.47693207 10-08-20 30.7000 0.00209886552 1543.626764
## 30    9 7.75308521 10-08-20 31.3000 0.00206630891  773.137684
## 31   10 7.47649394 10-08-20 30.7000 0.00205467181 1512.443403
## 32   11 7.69375960 10-08-20 31.0000 0.00200576246  870.043423
## 33    3 7.77077703 11-08-20 30.4500 0.00207103545  745.953016
## 35    8 7.46807316 11-08-20 30.5000 0.00209886552 1578.578400
## 36    9 7.77117000 11-08-20 30.8000 0.00206630891  741.699095
## 37   10 7.43647817 11-08-20 30.9000 0.00205467181 1662.562703
## 38   11 7.68217235 11-08-20 30.9000 0.00200576246  895.713549
## 39    3 7.79721822 12-08-20 30.8375 0.00207103545  696.611452
## 41    8 7.49340983 12-08-20 30.7500 0.00209886552 1483.374915
## 42    9 7.83260159 12-08-20 31.0000 0.00206630891  635.437845
## 43   10 7.49189124 12-08-20 31.0250 0.00205467181 1454.875543
## 44   11 7.79020674 12-08-20 31.2500 0.00200576246  684.239085
## 45    3 7.75200968 20-08-20 31.6000 0.00207103545  775.510239
## 46    6 7.48356129 20-08-20 31.9000 0.00205107662 1474.627785
## 47    8 7.52057315 20-08-20 31.9000 0.00209886552 1380.721981
## 48    9 7.76789521 20-08-20 31.2000 0.00206630891  745.744648
```

```
## 49   10 7.61627621 20-08-20 32.6000 0.00205467181 1067.678967
## 50   11 7.73904235 20-08-20 33.0000 0.00200576246  768.781355
```