Exploratory Analysis

Tony Ni, Antonella Basso, Jose Lopez

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Libraries

Goals:

comparing how upgradients look vs downgradients through a graph (make sure the average thing/wrangling to fix it)

pick a chemical of interest

histograms of concentrations (one for upgradient vs downgradient for a single site)

compare the compare the 2 powerplants overall (upgradient at one vs the other)

regression

Reading in Data

```
setwd("~/harvard-summer-biostats")
illinois <- read_csv("data/illinois.csv") #read in data
```

```
## Warning: Missing column names filled in: 'X1' [1]
```

```
## Parsed with column specification:
## cols(
##   X1 = col_double(),
##   state = col_character(),
##   site = col_character(),
##   disposal.area = col_character(),
##   type = col_character(),
##   well.id = col_character(),
##   gradient = col_character(),
##   samp.date = col_character(),
##   contaminant = col_character(),
##   measurement.unit = col_character(),
##   concentration = col_double()
## )
```

Checking unique/distinct levels

```r
#check how many observations there
nrow(illinois)
```

```
## [1] 38792
```

```r
#checking distincts sites
unique(illinois$site)
```

```
##  [1] "Baldwin Energy Complex"
##  [2] "Coffeen Power Station"
##  [3] "Dallman Power Generating Station"
##  [4] "Duck Creek Power Station"
##  [5] "Edwards Power Station"
##  [6] "Havana Power Station"
##  [7] "Hennepin Power Station"
##  [8] "Joliet #29 Generating Station"
##  [9] "Joliet #9 Generating Station"
## [10] "Joppa Power Station"
## [11] "Kincaid Power Station"
## [12] "Newton Power Station"
## [13] "Powerton Generating Station"
## [14] "Prairie State Generating Company, LLC"
## [15] "SIPC Marion Power Plant"
## [16] "Waukegan Station"
## [17] "Will County"
## [18] "Wood River Power Station"
```

```r
#checking distinct gradient
unique(illinois$gradient)
```

```
## [1] "Downgradient" "Upgradient"   "Unknown"
```

```r
#checking distinct gradient
unique(illinois$measurement.unit)
```

```
## [1] "mg/l"  "su"    "pCi/l" "ug/l"
```

```r
#checking disposal area
unique(illinois$disposal.area)
```

```
##  [1] "Baldwin Bottom Ash Pond"
##  [2] "Baldwin Fly Ash Pond System"
##  [3] "Baldwin Bottom Ash Pond, Baldwin Fly Ash Pond System"
##  [4] "Coffeen Ash Pond No. 2"
##  [5] "Coffeen Ash Pond No. 1"
##  [6] "Coffeen GMF Recycle Pond"
##  [7] "Coffeen GMF Gypsum Stack Pond"
##  [8] "Coffeen GMF Gypsum Stack Pond, Coffeen Landfill"
##  [9] "Coffeen Ash Pond No. 1, Coffeen Ash Pond No. 2"
## [10] "Coffeen Landfill"
```

```
## [11] "Coffeen Ash Pond No. 2, Coffeen GMF Recycle Pond"
## [12] "Dallman Ash Pond, Lakeside Ash Pond"
## [13] "Duck Creek Bottom Ash Basin"
## [14] "Duck Creek Landfill"
## [15] "Duck Creek GMF Pond"
## [16] "Edwards Ash Pond"
## [17] "Havana East Ash Pond (Cells 1, 2, 3, and 4)"
## [18] "Hennepin Ash Pond No. 2, Hennepin East Ash Pond, Hennepin Landfill"
## [19] "Henepin Old West Ash Pond (Pond No. 1 and Pond No. 3) and Hennepin Old West Polishing Pond"
## [20] "Hennepin Ash Pond No. 2"
## [21] "Hennepin East Ash Pond"
## [22] "Hennepin Landfill"
## [23] "Ash Pond 2"
## [24] "Lincoln Stone Quarry"
## [25] "Joppa Landfill"
## [26] "Joppa East Ash Pond"
## [27] "Kincaid Ash Pond"
## [28] "Newton Landfill 2"
## [29] "Newton Primary Ash Pond"
## [30] "Ash By-pass Basin, Ash Surge Basin, Former Ash Basin"
## [31] "Near Field Landfill"
## [32] "Settling Pond"
## [33] "West Ash Pond, East Ash Pond"
## [34] "Ash Pond 2 South, Ash Pond  3 South"
## [35] "Wood River West Ash Ponds 1, 2E, 2W"
## [36] "Wood River Primary East Ash Pond"
```

```
#checking type (L = land fuel, SI = surface impoundement, M = mixed/multiunit)
#there will be multiple different dumpsites at a powerplant site. some sites are wet (ponds of water wh
unique(illinois$type)
```

```
## [1] "SI" "M"  "L"
```

```
illinois %>%
  group_by(type) %>%
  summarize(n())
```

```
## # A tibble: 3 x 2
##   type  `n()`
##   <chr> <int>
## 1 L      8869
## 2 M       875
## 3 SI    29048
```

```
illinois %>%
  group_by(measurement.unit) %>%
  summarize(n())
```

```
## # A tibble: 4 x 2
##   measurement.unit `n()`
##   <chr>            <int>
## 1 mg/l             32526
```

```
## 2 pCi/l             1721
## 3 su                1964
## 4 ug/l              2581
```

```
#checking wells
illinois %>%
  group_by(well.id) %>%
  summarize(n())
```

```
## # A tibble: 198 x 2
##    well.id `n()`
##    <chr>   <int>
##  1 03R       175
##  2 05DR      175
##  3 05R       175
##  4 08D       175
##  5 12        175
##  6 13        175
##  7 18D       175
##  8 18S       172
##  9 2         174
## 10 21        350
## # ... with 188 more rows
```

use illinois and newyork

lower detection limit (if a chemical is really low, it can't differentiate beyond a certain low level, it might be the values with all teh same values)

all of the contaminants are harmful, some chemicals are more useful for detecting coal contamination (most important/indicative of coal contamination is boron (occurs at really high levels in coal)),

looking at the report given to us might be good about the different chemicals in coal (if we are curious)

total dissolved solids are probably not important, imprevise measurement of how much "crap is in the water" - doesnt represent any toxic chemicals

Wrangling

```
illinois1 <- illinois %>%
  select(site, disposal.area, type, well.id, gradient, contaminant,
         measurement.unit, concentration) %>%
  mutate(well.id_contaminant = paste0(well.id, "_", contaminant)) %>% #for future use
  rename(c("disposal_area" = "disposal.area", "well_id" = "well.id",
           "unit" = "measurement.unit"))

#fixing 'contaminant' string by removing everything after the comma
illinois1$contaminant=gsub(", total", "", illinois1$contaminant)

#testing
avg_contaminant <- illinois1 %>%
  group_by(well_id, contaminant) %>%
  summarise_each(funs(mean)) %>%
```

```
  select(1,2,8) #selecting only numeric columns

#temporarily uniting columns for joining in next step
temp <- avg_contaminant %>%
  unite("well.id_contaminant", well_id, contaminant)

#joining orig dataframe and avg_contaminant dataframe
combined <- left_join(temp, illinois1, by = "well.id_contaminant") %>%
  distinct(well.id_contaminant, .keep_all = TRUE) %>%
  separate(well.id_contaminant, c('well_id', 'contaminant'), sep="_") %>%
  select(1:8)

#spreading to wide data frame format to add missing info
combined2 <- combined %>% #collapse empty rows
  spread(contaminant, concentration.x) %>%
  group_by(well_id) %>%
  summarise_each(funs(first(.[!is.na(.)]))) %>%
  select(-c(unit))

#gathering back to long data frame format
combined3 <- combined2 %>%
  gather("contaminant", "concentration", 6:26)
```

Summary Statistics

```
illinois %>%
  group_by(contaminant) %>%
  summarize(mean_concentration = mean(concentration))
```

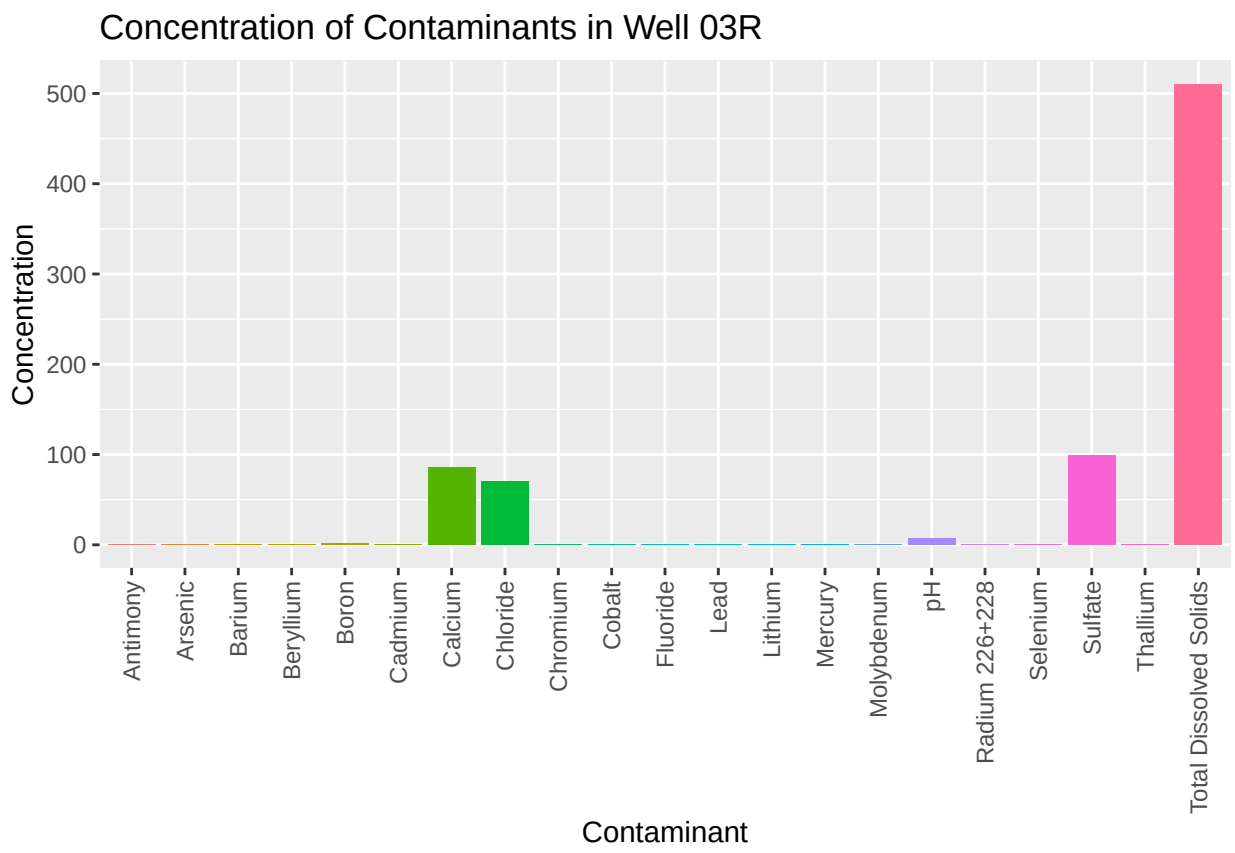
```
## # A tibble: 21 x 2
##    contaminant      mean_concentration
##    <chr>                         <dbl>
##  1 Antimony, total               0.626
##  2 Arsenic, total                2.56
##  3 Barium, total                39.8
##  4 Beryllium, total              0.141
##  5 Boron, total                125.
##  6 Cadmium, total                0.141
##  7 Calcium, total             7460.
##  8 Chloride                     79.1
##  9 Chromium, total               0.969
## 10 Cobalt, total                 0.761
## # ... with 11 more rows
```

Visualizations

```
#looking at one specific well and the contaminant concentrations within it

ggplot(data = combined3 %>%
```

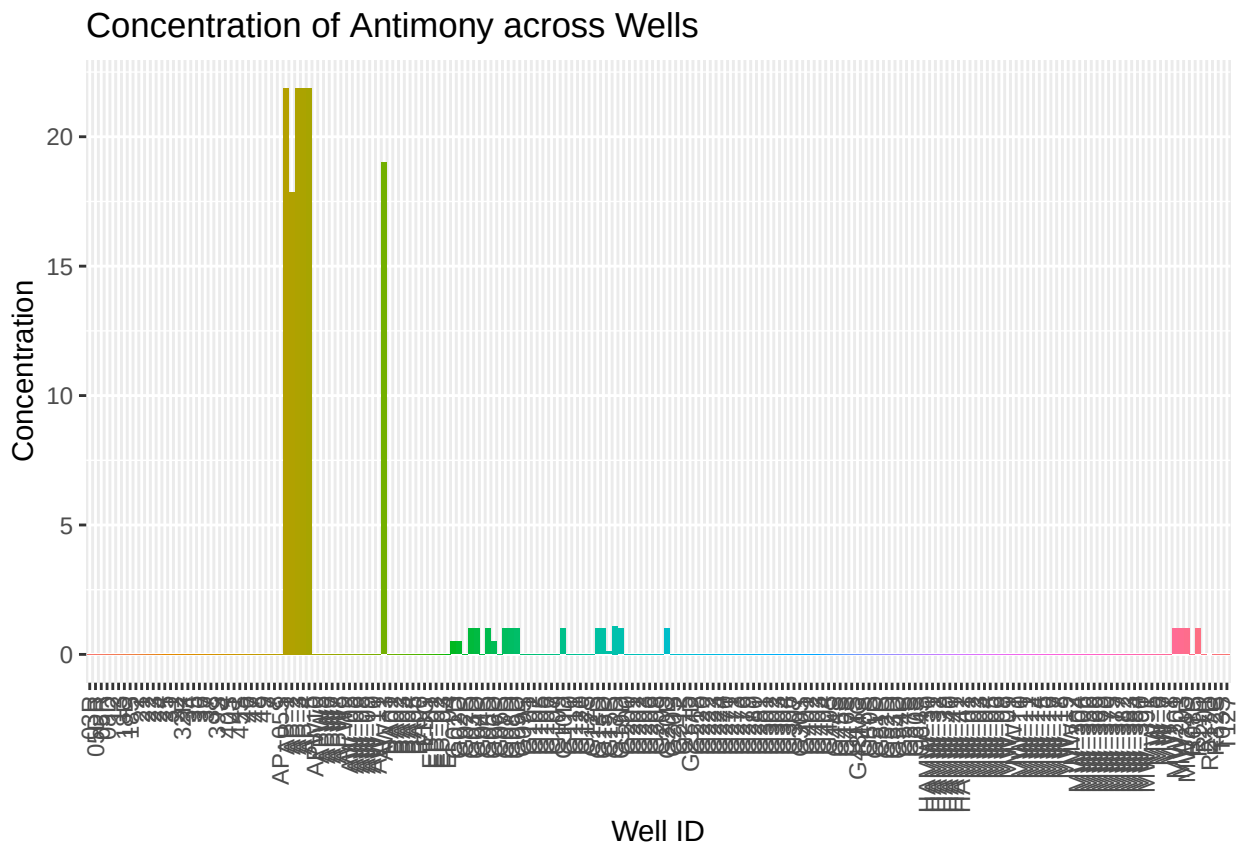
```
        filter(well_id == "03R"), aes(x = contaminant, y = concentration,
                                      fill = contaminant)) +
  geom_bar(stat = "identity", show.legend = FALSE) +
  xlab("Contaminant") +
  ylab("Concentration") +
  ggtitle("Concentration of Contaminants in Well 03R") +
  theme(axis.text.x = element_text(angle = 90, vjust = 0.5, hjust=1))
```




```
#looking at one contaminant for all wells (counts)

ggplot(data = combined3 %>%
         filter(contaminant == "Antimony"),
       aes(x = well_id, y = concentration, fill = well_id)) +
  geom_bar(stat = "identity", show.legend = FALSE) +
  xlab("Well ID") +
  ylab("Concentration") +
  ggtitle("Concentration of Antimony across Wells") +
  theme(axis.text.x = element_text(angle = 90, vjust = 0.5, hjust=1))
```

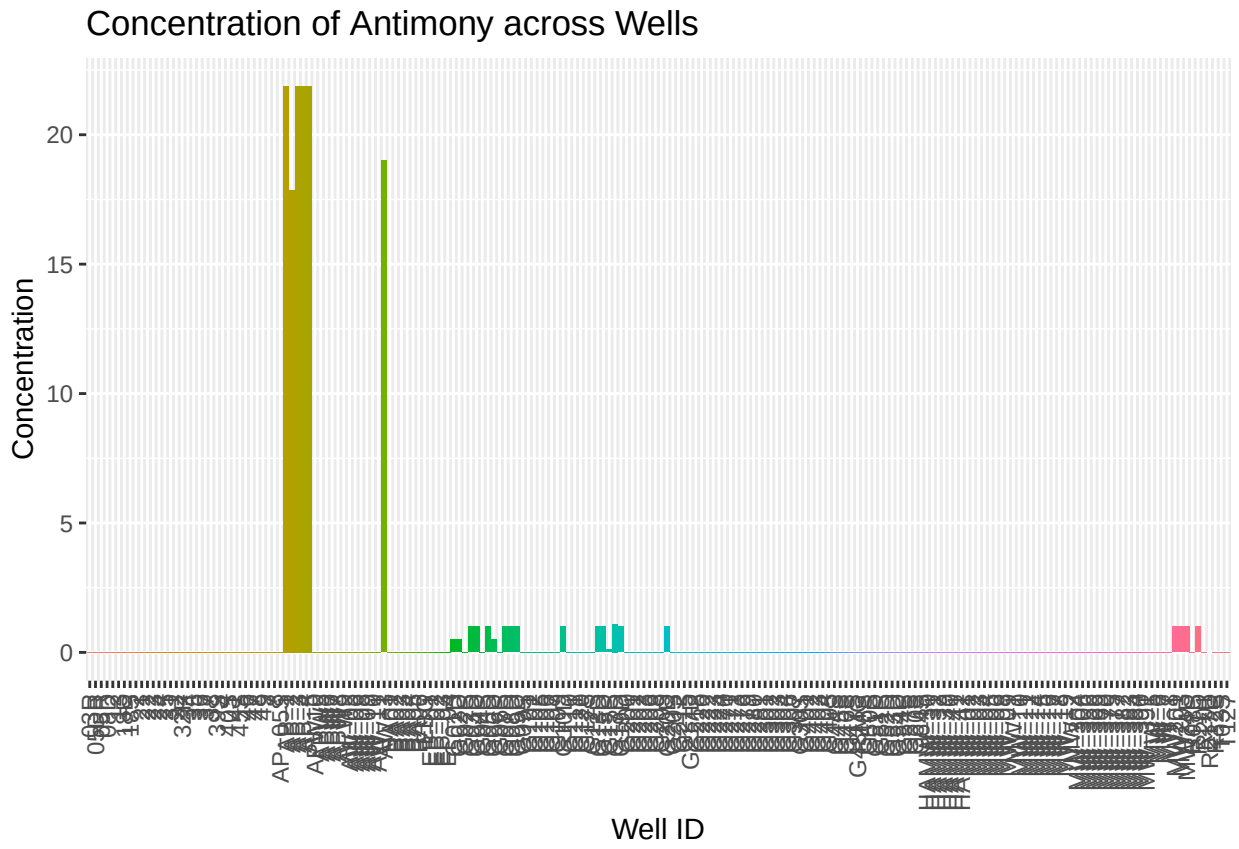
```
## Warning: Removed 1 rows containing missing values (position_stack).
```



The histogram is incompehensible, there are way too many wells in Illinois. Unsure, but having to make all these plots constantly seems unreasonable for all of these potential wells and contaminants to look through, maybe choose only those wells with concentration values greater than some certain value? (0.001 maybe?)

```
ggplot(data = combined3 %>%
         filter(contaminant == "Antimony"),
       aes(x = well_id, y = concentration, fill = well_id)) +
  geom_bar(stat = "identity", show.legend = FALSE) +
  xlab("Well ID") +
  ylab("Concentration") +
  ggtitle("Concentration of Antimony across Wells") +
  theme(axis.text.x = element_text(angle = 90, vjust = 0.5, hjust=1))
```

```
## Warning: Removed 1 rows containing missing values (position_stack).
```




```
levels(as.factor(combined3$well_id))
```

```
##   [1] "03R"     "05DR"    "05R"     "08D"     "12"      "13"      "18D"
##   [8] "18S"     "2"       "21"      "22"      "23"      "24"      "25"
##  [15] "31"      "32"      "32R"     "34"      "35"      "36"      "37"
##  [22] "38"      "39S"     "4"       "40S"     "41"      "45S"     "46"
##  [29] "47"      "48"      "49"      "7"       "8"       "AP-05S"  "AP-1"
##  [36] "AP-2"    "AP-3"    "AP-4"    "AP-5"    "APW10"   "APW5"    "APW6"
##  [43] "APW7"    "APW8"    "APW9"    "AW-05"   "AW-06"   "AW-08"   "AW-09"
##  [50] "AW-10"   "AW-11"   "AW-3"    "BA01"    "BA02"    "BA03"    "BA04"
##  [57] "BA05"    "BA06"    "EBG"     "EP-01"   "EP-02"   "EP-03"   "EP-04"
##  [64] "G01D"    "G02D"    "G02S"    "G03D"    "G04D"    "G04S"    "G05D"
##  [71] "G06D"    "G06S"    "G07D"    "G08D"    "G09D"    "G09S"    "G101"
##  [78] "G102"    "G105"    "G106"    "G107"    "G109"    "G10D"    "G110"
##  [85] "G111"    "G120"    "G125"    "G12S"    "G13D"    "G15D"    "G15S"
##  [92] "G17D"    "G19D"    "G200"    "G201"    "G202"    "G203"    "G206"
##  [99] "G208"    "G209"    "G20D"    "G20S"    "G212"    "G215"    "G217D"
## [106] "G218"    "G220"    "G222"    "G223"    "G224"    "G270"    "G271"
## [113] "G273"    "G276"    "G279"    "G280"    "G281"    "G301"    "G302"
## [120] "G303"    "G304"    "G306"    "G307"    "G30S"    "G401"    "G402"
## [127] "G403"    "G404"    "G405"    "G44S"    "G45S"    "G46S"    "G47S"
## [134] "G48MG"   "G48S"    "G50S"    "G51D"    "G51S"    "G52D"    "G53D"
## [141] "G54D"    "G54S"    "G57S"    "G60S"    "G64S"    "HAMW-30" "HAMW-31"
## [148] "HAMW-32" "HAMW-39" "HAMW-40" "HAMW-41" "HAMW-42" "MW-01"   "MW-02"
## [155] "MW-03"   "MW-04"   "MW-05"   "MW-06"   "MW-08"   "MW-09"   "MW-1"
```

```
## [162] "MW-10"   "MW-11"   "MW-12"   "MW-14"   "MW-15"   "MW-16"   "MW-17"
## [169] "MW-18"   "MW-19"   "MW-2"    "MW-304"  "MW-306"  "MW-356"  "MW-366"
## [176] "MW-369"  "MW-370"  "MW-375"  "MW-377"  "MW-382"  "MW-383"  "MW-384"
## [183] "MW-390"  "MW-391"  "MW-5"    "MW-6"    "MW-7"    "MW-8"    "MW201"
## [190] "MW203"   "MW24D"   "R08S"    "R11D"    "R201"    "R217D"   "R32S"
## [197] "T03S"    "T127"
```

#Comparing Upgradient Wells

```
#get the first 10 highest avg mg/l (not ph or total sulfate)
#not pH, total dissolve solids, or radium b/c different units

dont_use <- c("pH", "Radium 226+228", "Total Dissolved Solids")

#pull out the names (from top 10 high to low avg concentrations) of contaminants
chemicals <- combined3 %>%
    filter(contaminant != "pH") %>% #take our nonuseful contaminants
  filter(contaminant != "Radium 226+228") %>%
  filter(contaminant != "Total Dissolved Solids") %>%
    group_by(contaminant) %>%
    summarise(avg_conc = mean(concentration)) %>%
    arrange(desc(avg_conc)) %>%
  slice(1:10) %>% #there only seem to be 5 chemicals of nonzero(basically) values
    pull(contaminant)

chemicals
```

```
##  [1] "Calcium"   "Sulfate"   "Boron"     "Chloride"  "Fluoride"  "Antimony"
##  [7] "Arsenic"   "Barium"    "Beryllium" "Cadmium"
```

```
combined3 %>%
    filter(contaminant != "pH") %>% #take our nonuseful contaminants
  filter(contaminant != "Radium 226+228") %>%
  filter(contaminant != "Total Dissolved Solids") %>%
    group_by(contaminant) %>%
    summarise(avg_conc = mean(concentration))
```

```
## # A tibble: 18 x 2
##    contaminant avg_conc
##    <chr>          <dbl>
##  1 Antimony      NA
##  2 Arsenic       NA
##  3 Barium        NA
##  4 Beryllium     NA
##  5 Boron        145.
##  6 Cadmium       NA
##  7 Calcium     8142.
##  8 Chloride      75.3
##  9 Chromium      NA
## 10 Cobalt        NA
## 11 Fluoride       0.459
## 12 Lead          NA
## 13 Lithium       NA
```

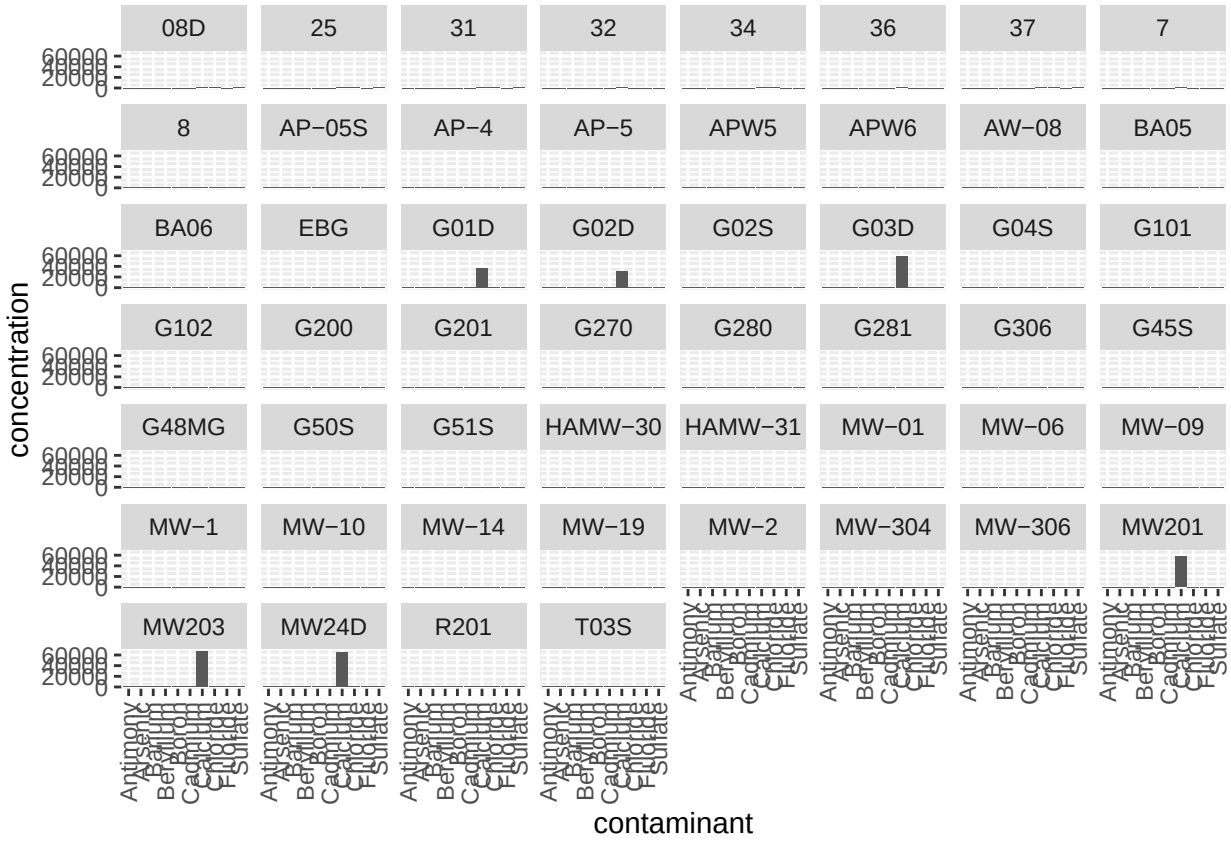
```
## 14 Mercury       NA
## 15 Molybdenum    NA
## 16 Selenium      NA
## 17 Sulfate      204.
## 18 Thallium      NA
```

Is doing the mean of concentrations amongst all wells OK to do? Some wells like arsenic have wells with 0.001 (sign that measurement was insignificant/below threshold), and taking the avg sometimes makes it return NA as the mean (I THINK??? what does NA mean...?) ASK LULI (i think some of the chemicals in the paper had thresholds of DANGER that were in mg and others in microg, how would we account for this...?)

https://postimg.cc/ZCc072JM

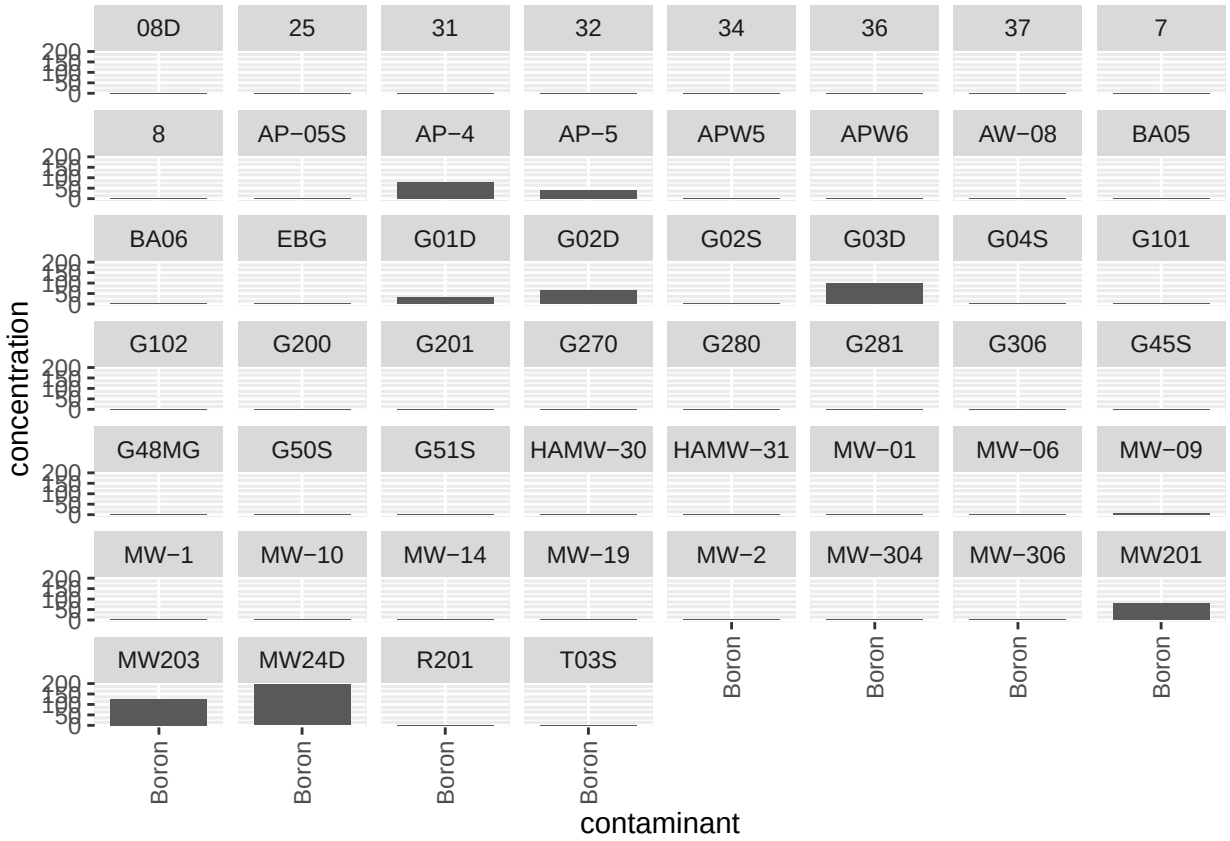
Do the blank entries (Calcium, Chloride, Fluoride, etc.) mean that they are non toxic/naturally occuring?

```
#plot in a faceted grid bar plots of concentration vs. contaminant for all wells
ggplot(data = combined3 %>%
        filter(gradient == "Upgradient") %>%
        filter(contaminant %in% chemicals),
      aes(x = contaminant, y = concentration)) +
      geom_bar(stat = "Identity") +
      facet_wrap(well_id ~ .) +
      theme(axis.text.x = element_text(angle = 90, vjust = 0.5, hjust=1))
```

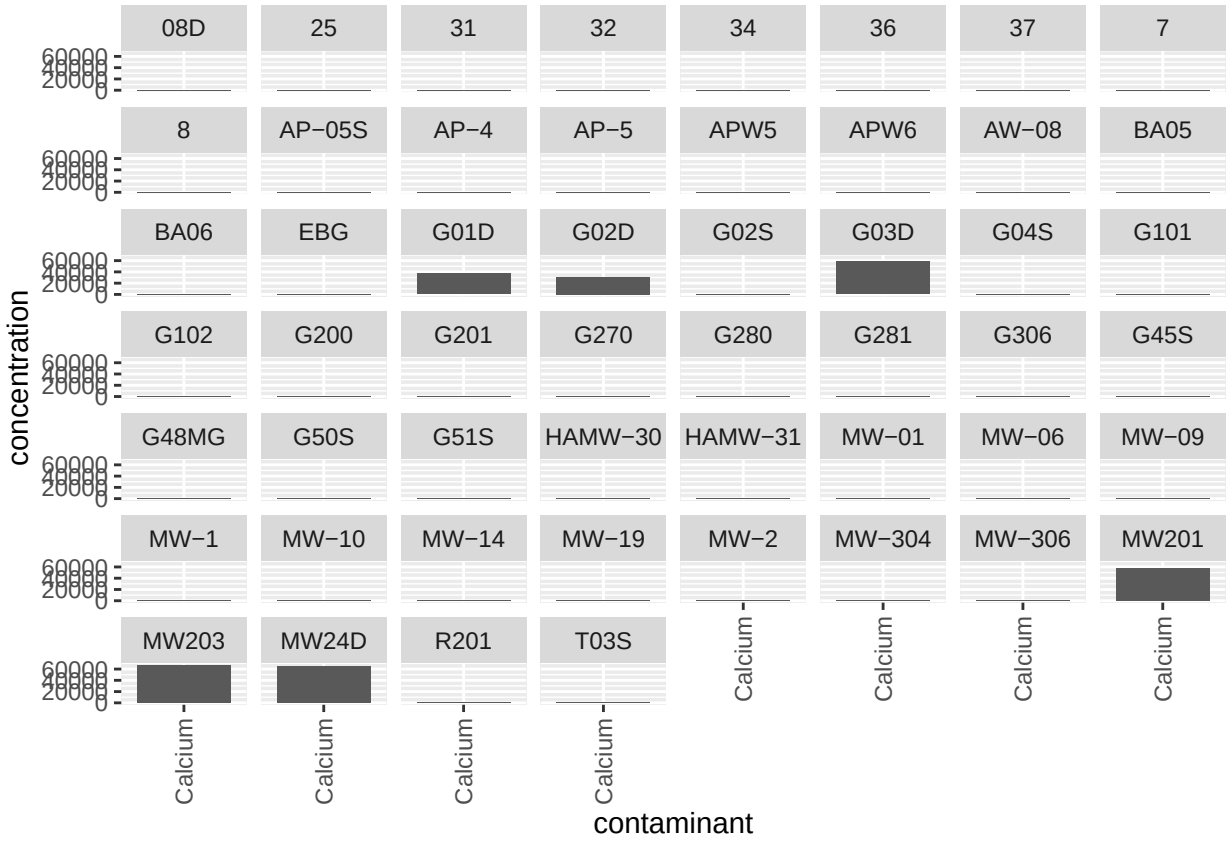


The concentration of calcium is so high in some of the wells, it makes it difficult to look at the other contaminants' concentration across all wells, perhaps we should make different facetted plots for all contaminants.

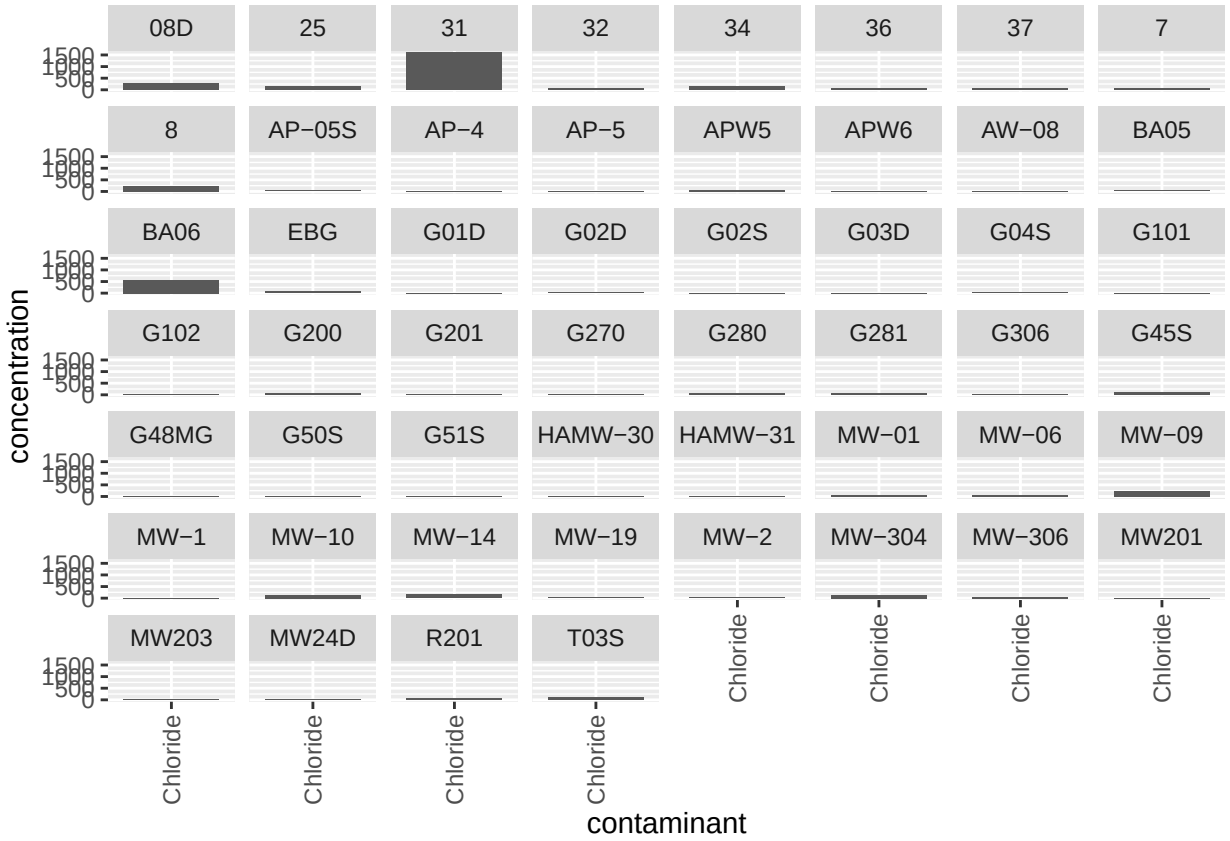
```
#Boron
ggplot(data = combined3 %>%
         filter(gradient == "Upgradient") %>%
         filter(contaminant %in% chemicals) %>%
         filter(contaminant == "Boron"),
       aes(x = contaminant, y = concentration)) +
       geom_bar(stat = "Identity") +
       facet_wrap(well_id ~ .) +
       theme(axis.text.x = element_text(angle = 90, vjust = 0.5, hjust=1))
```



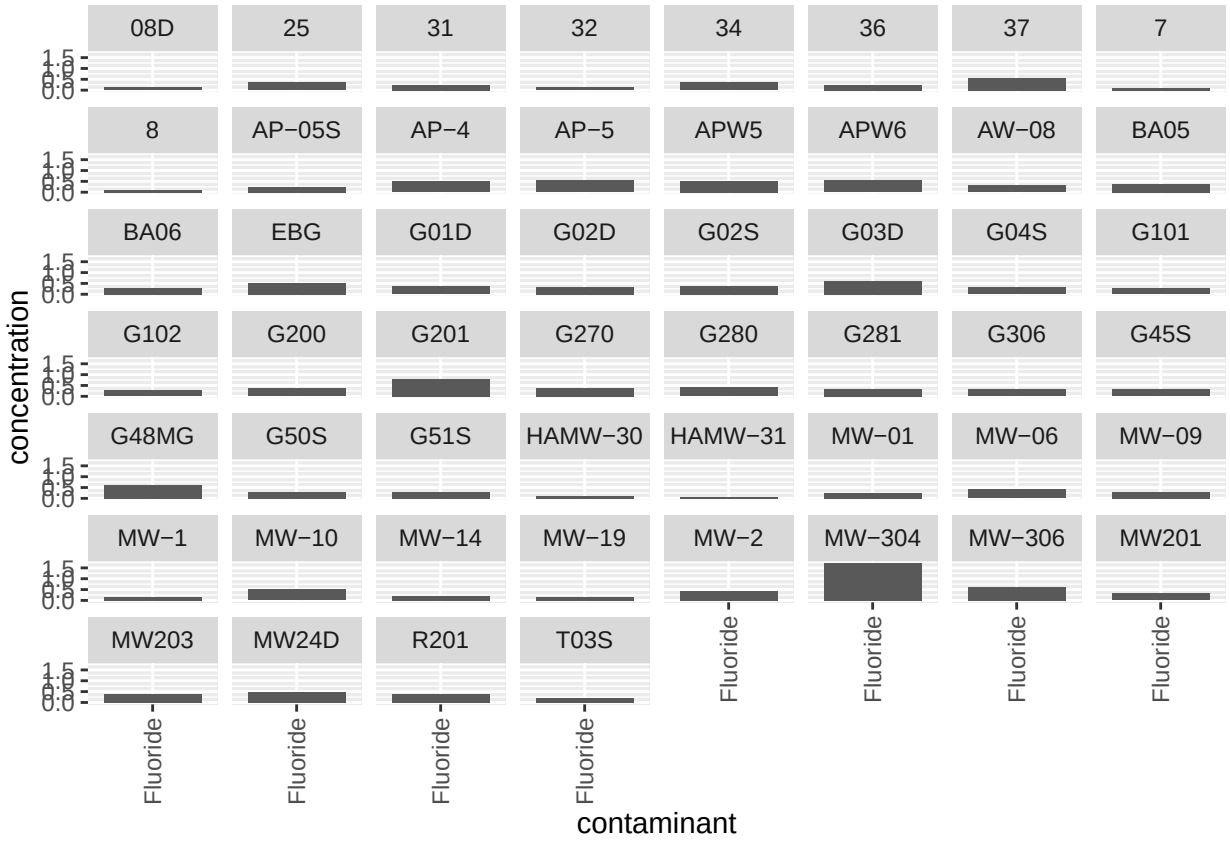

```
#Calcium
ggplot(data = combined3 %>%
         filter(gradient == "Upgradient") %>%
         filter(contaminant %in% chemicals) %>%
         filter(contaminant == "Calcium"),
       aes(x = contaminant, y = concentration)) +
       geom_bar(stat = "Identity") +
       facet_wrap(well_id ~ .) +
       theme(axis.text.x = element_text(angle = 90, vjust = 0.5, hjust=1))
```



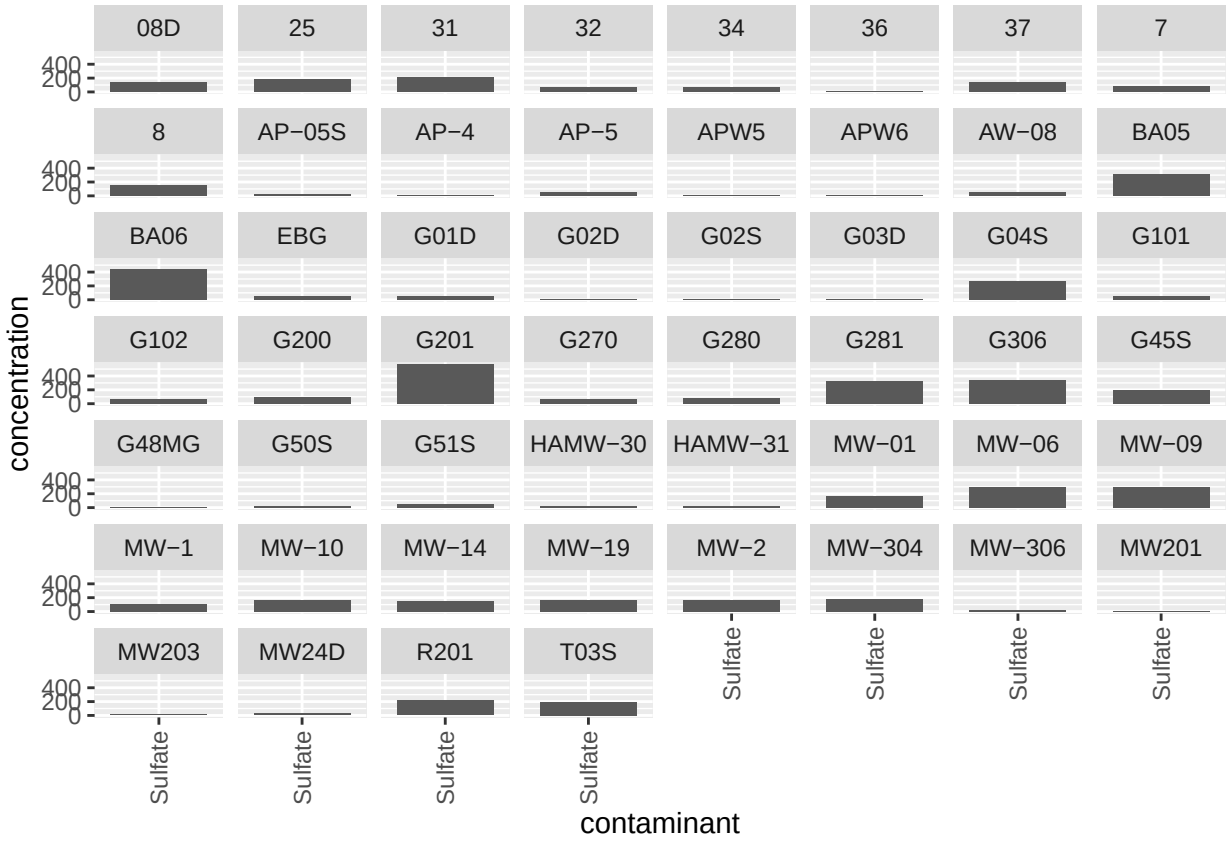

```
#Chloride
ggplot(data = combined3 %>%
         filter(gradient == "Upgradient") %>%
         filter(contaminant %in% chemicals) %>%
         filter(contaminant == "Chloride"),
       aes(x = contaminant, y = concentration)) +
       geom_bar(stat = "Identity") +
       facet_wrap(well_id ~ .) +
       theme(axis.text.x = element_text(angle = 90, vjust = 0.5, hjust=1))
```




```
#Fluoride
ggplot(data = combined3 %>%
         filter(gradient == "Upgradient") %>%
         filter(contaminant %in% chemicals) %>%
         filter(contaminant == "Fluoride"),
       aes(x = contaminant, y = concentration)) +
       geom_bar(stat = "Identity") +
       facet_wrap(well_id ~ .) +
       theme(axis.text.x = element_text(angle = 90, vjust = 0.5, hjust=1))
```



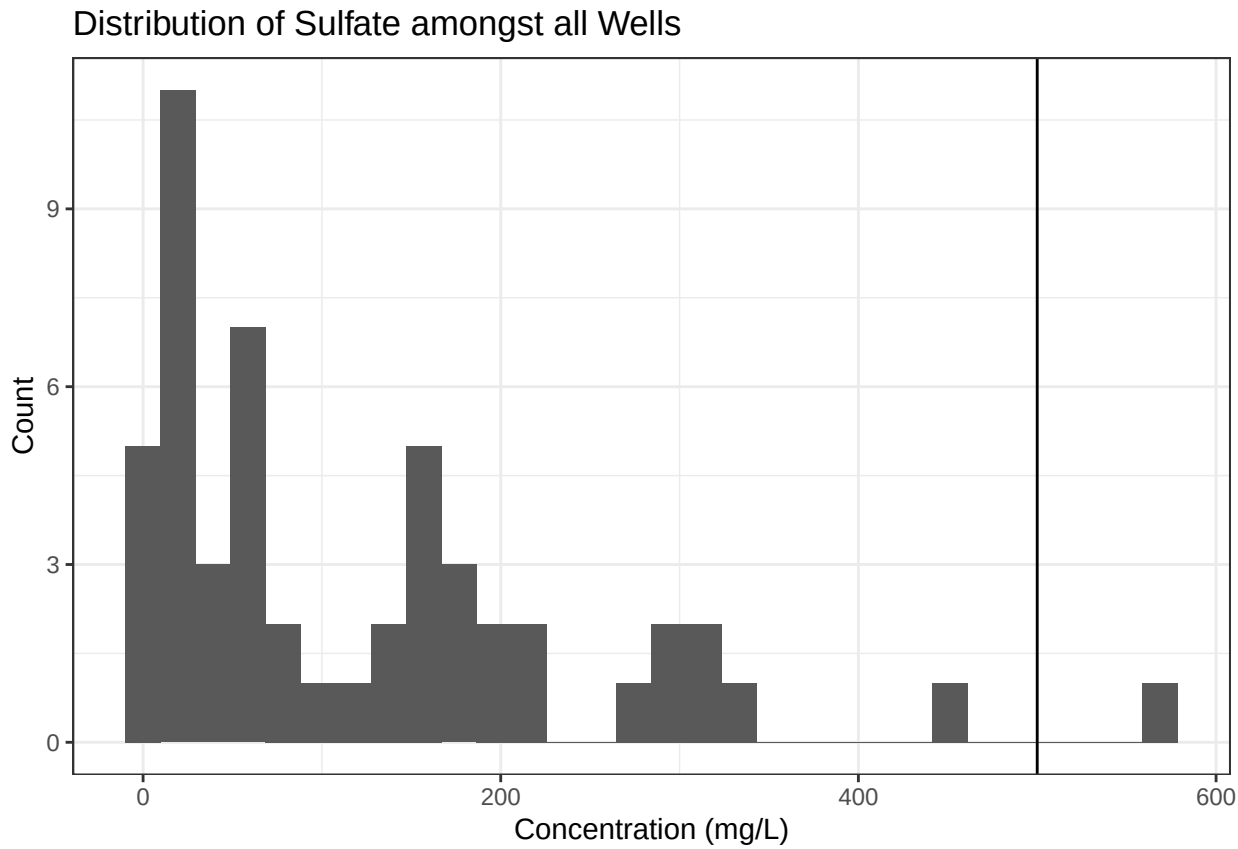

```
#Sulfate
ggplot(data = combined3 %>%
         filter(gradient == "Upgradient") %>%
         filter(contaminant %in% chemicals) %>%
         filter(contaminant == "Sulfate"),
       aes(x = contaminant, y = concentration)) +
       geom_bar(stat = "Identity") +
       facet_wrap(well_id ~ .) +
       theme(axis.text.x = element_text(angle = 90, vjust = 0.5, hjust=1))
```



Let's make a histogram to show distribution of certain contaminants:

```
#Sulfate
ggplot(data = combined3 %>%
         filter(gradient == "Upgradient") %>%
         filter(contaminant %in% chemicals) %>%
         filter(contaminant == "Sulfate"),
       aes(x = concentration)) +
       geom_histogram() +
       geom_vline(xintercept = 500) + #threshold value
  xlab("Concentration (mg/L)") +
  ylab("Count") +
  ggtitle("Distribution of Sulfate amongst all Wells") +
  theme_bw()
```

```
## `stat_bin()` using `bins = 30`. Pick better value with `binwidth`.
```



How do we determine what is the NORM? What would the usual distribution of sulfate be if it were not contaminated?

Comments/Notes Below:

we could see that in an exploratory analysis, look at histogram of different chemcials at each well – there should be variation btwn upgradients at the same sites and general amt of different between upgradient at one site vs another site... one source of variation is the site and wells will also have some variation in their measurement too... make histograms for all chemcials and visualize them side by side and see if theres any differnces between upgradients and downgradients, and check if any differences between upgradients.. statistically there is a way... group them by upgradient vs downgradient (groupby chemicals and plot x variable concentration, and facet by the gradient (either up or down) and get histograms for each)

In the powerpoint, it talks about comparing upgradient wells within 100 mi radius of each other, how should we go about getting this distance data since it isn't provided? Should we try to use outside data/geospatial data to do this?

> For now, looking at data w/o distance probably is fine – we might incorporate distance if we get further/have time.

Are all the contaminants which are being measured of danger? Or are there only certain ones that should be looked at which are dangerous?

I realized a lot of the values are inconsistent in their units, some are ug/L others of mg/L, etc. It would be nice to standardize these across the board in the pre-wrangling stage...

> http://www.eai-labs.com/assets/docs/radioactive_in_water.pdf says "micrograms per liter (ug/L) can be converted to pCi/L by multiplying the U (mg/L) by 0.67"

Plot 1: Compare concentrations at a small number of upgradient wells with other upgradient wells at the same site.

Looking at https://www.uky.edu/KGS/coal/coal-major-minor-trace-elements.php , we find that the major elements in coal consist of: Hydrogen, Carbon, Nitrogen, Oxygen, and Sulfur with the minor elements in coal being: Sodium, Aluminum, Silicon, Phosphorous, Potassium, Calcium, Titanium, Manganese, and Iron

The contaminants being measured in our case are Sulfate (a compound containing sulfur), Calcium,