Chemical EDA

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```
# Read in the cleaned dataset and select records of California and Florida
df <- read.csv("strawberry_cleaned.csv")

# Find states that used chemicals in growing strawberry
states_with_chemical_info <- df %>%
  filter(!is.na(Chemical_Info)) %>%
  distinct(State) %>%
  pull(State)

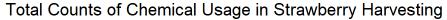
print(states_with_chemical_info)
```

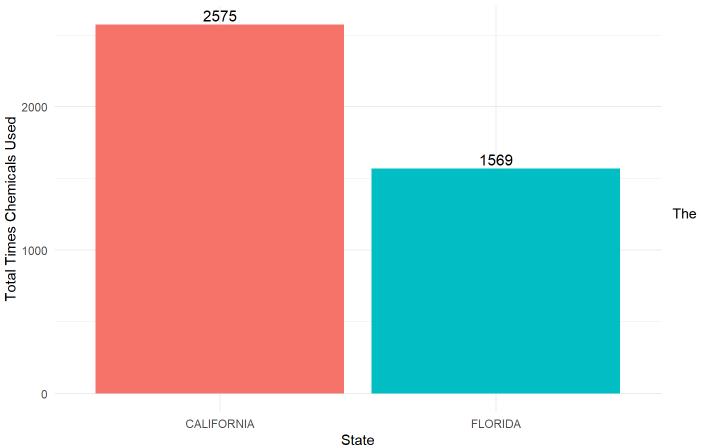
```
## [1] "CALIFORNIA" "FLORIDA"
```

Only California and Florida used chemicals when growing strawberries, we can filter out only those two states and compare the frequency of chemical used:

```
df1 <- df %>%
  select(-1) %>%
  filter(State == "CALIFORNIA" | State == "FLORIDA")

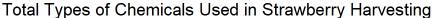
# Draw a bar plot comparing the frequency
chem_state <- df1 %>%
  group_by(State) %>%
  summarise(Total_obs=n()) %>%
  arrange(desc(Total_obs))
print(chem_state)
```





frequency that California used chemicals is almost twice as the frequency of Florida.

```
# Split the California data and Florida data into two dataframes
df_cal <- df %>%
  filter(State == "CALIFORNIA")
df_flo <- df %>%
  filter(State == "FLORIDA")
# Find the distinct chemicals used in California and Florida
chem_comparison <- data.frame(</pre>
  State = c("CALIFORNIA", "FLORIDA"),
  Distinct_chemicals =
    c(length(unique(df_cal$Chemical_Info)),
      length(unique(df_flo$Chemical_Info)))
)
ggplot(chem_comparison, aes(x = State, y = Distinct_chemicals, fill = State)) +
  geom_bar(stat = "identity") +
  geom_text(aes(label = Distinct_chemicals), vjust = -0.3, size = 4) +
  theme_minimal() +
  labs(title = "Total Types of Chemicals Used in Strawberry Harvesting",
       x = "State",
       y = "Total Types of Chemicals Used") +
  theme(legend.position = "none") # Remove Legend
```





finding the distinct chemicals in each state, California used 19 more types of chemicals than Florida, and there are 58 types of chemicals used in California but not in Florida:

```
# Find out chemicals used by California but not used by Florida
diff_chem1 <- setdiff(unique(df_cal$Chemical_Info), unique(df_flo$Chemical_Info))
print(diff_chem1)</pre>
```

- ## [1] "CYCLANILIPROLE" [2] "PERMETHRIN" ## [3] "ISARIA FUMOSOROSEA STRAIN FE 9901" [4] "BACILLUS AMYLOLIQUEFACIENS STRAIN D747" ## [5] "BLAD" ## [6] "BT SUBSP KURSTAKI EVB-113-19" ## ## [7] "POLYOXIN D ZINC SALT" [8] "QUINOLINE" ## [9] "TRIFLOXYSTROBIN" ## ## [10] "PENDIMETHALIN" ## [11] "ACEQUINOCYL" ## [12] "AZADIRACHTIN" ## [13] "BEAUVERIA BASSIANA" ## [14] "BT KURSTAKI SA-11" ## [15] "CANOLA OIL" ## [16] "CHROMOBAC SUBTSUGAE PRAA4-1 CELLS AND SPENT MEDIA" ## [17] "ETOXAZOLE" ## [18] "FENBUTATIN-OXIDE" ## [19] "NEEM OIL" ## [20] "NEEM OIL, CLAR. HYD." ## [21] "PYRIDABEN" ## [22] "CAPSICUM OLEORESIN EXTRACT" ## [23] "GARLIC OIL" ## [24] "IRON PHOSPHATE" ## [25] "METALDEHYDE" ## [26] "METAM-SODIUM" ## [27] "BACILLUS AMYLOLIQUEFACIENS MBI 600" ## [28] "BACILLUS PUMILUS" ## [29] "COPPER OCTANOATE" ## [30] "POTASSIUM BICARBON." ## [31] "STREPTOMYCES LYDICUS" ## [32] "BT KURSTAKI EG7841" ## [33] "BT SUB AIZAWAI GC-91" ## [34] "BUPROFEZIN" ## [35] "BURKHOLDERIA A396 CELLS & MEDIA" ## [36] "HELICOVERPA ZEA NPV" ## [37] "PETROLEUM DISTILLATE" ## [38] "POTASSIUM SALTS" ## [39] "PYRIPROXYFEN" ## [40] "CAPRIC ACID" ## [41] "CAPRYLIC ACID" ## [42] "MINERAL OIL" ## [43] "PAECILOMYCES FUMOSOR" ## [44] "POTASSIUM SILICATE" ## [45] "BACILLUS SUBT. GB03" ## [46] "TRICHODERMA HARZ." ## [47] "GLUFOSINATE-AMMONIUM" ## [48] "SULFENTRAZONE" ## [49] "CHLORPYRIFOS" ## [50] "SOYBEAN OIL" ## [51] "ZETA-CYPERMETHRIN"
- file:///C:/Users/sh/Documents/strawberry-assignment/chemical_eda.html

[52] "AUREOBASIDIUM PULLULANS DSM 14940"

```
## [53] "AUREOBASIDIUM PULLULANS DSM 14941"

## [54] "BT KURSTAKI SA-12"

## [55] "GLIOCLADIUM VIRENS"

## [56] "TRICHODERMA VIRENS STRAIN G-41"

## [57] "EMAMECTIN BENZOATE"

## [58] "SPIROTETRAMAT"
```

on the other hand, there are 39 types of chemicals used in Florida but not in California:

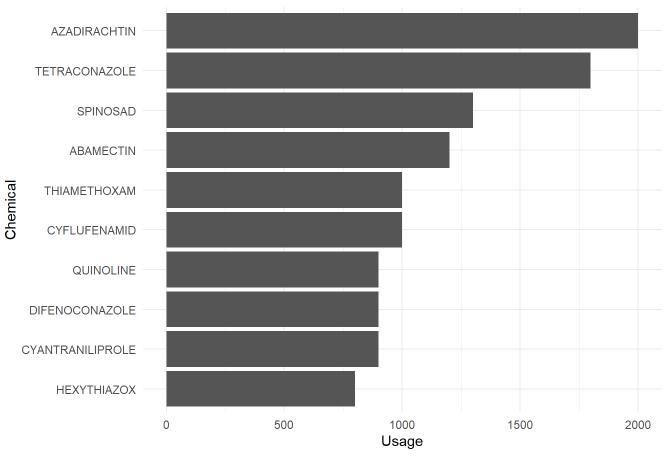
```
diff_chem2 <- setdiff(unique(df_flo$Chemical_Info), unique(df_cal$Chemical_Info))
print(diff_chem2)</pre>
```

```
[1] "PYRIOFENONE"
##
                                    "ZOXAMIDE"
##
   [3] "METSULFURON-METHYL"
                                    "PENOXSULAM"
##
   [5] "S-METOLACHLOR"
                                    "BETA-CYFLUTHRIN"
##
   [7] "ETHYL 2E;4Z-DECADIENOATE"
                                   "OXAMYL"
   [9] "CUPRAMMONIUM ACETATE"
                                    "DODECADIEN-1-OL"
## [11] "FLUENSULFONE"
                                    "GIBBERELLIC ACID"
                                    "COPPER CHLORIDE HYD."
## [13] "CHLOROTHALONIL"
## [15] "CYMOXANIL"
                                    "FAMOXADONE"
                                    "2,4-D, DIMETH. SALT"
## [17] "MANCOZEB"
## [19] "CLETHODIM"
                                    "METHOMYL"
## [21] "CYTOKININS"
                                    "INDOLEBUTYRIC ACID"
                                    "DIMETHENAMID"
## [23] "COPPER ETHANOLAMINE"
## [25] "FLUROXYPYR 1-MHE"
                                    "HALOSULFURON-METHYL"
                                    "FENAZAQUIN"
## [27] "KANTOR"
## [29] "ETHEPHON"
                                    "DODINE"
## [31] "FLUTOLANIL"
                                    "2,4-D, TRIISO. SALT"
## [33] "CYPERMETHRIN"
                                    "ALKYL. DIM. BENZ. AM"
                                    "DIDECYL DIM. AMMON."
## [35] "DECYLDIMETHYLOCTYL"
## [37] "DIMETHYLDIOCTYL"
                                    "MUSTARD OIL"
## [39] "DIMETHYL DISULFIDE DMDS"
```

We can first explore top chemicals used in California:

```
# Create a new column to record the frequency of each chemical used
chem_measure <- df_cal %>%
 group_by(Measurement) %>%
 filter(Measurement == "MEASURED IN LB")
# Plot the top chemicals used in California
top_chem <- chem_measure %>%
 filter(!is.na(Value)) %>%
 group_by(Chemical_Info, Domain) %>%
  summarise(Value = sum(Value, na.rm = TRUE)) %>%
 arrange(desc(Value))
ggplot(top_chem[1:10,],
       aes(x=reorder(Chemical_Info, Value), y=Value))+
 geom_bar(stat = "identity")+
 theme_minimal()+
 coord flip()+
 labs(x = "Chemical", y = "Usage",
       title = "Top 10 Chemicals Measured in LB in California")+
 theme(plot.title.position = "plot")
```

Top 10 Chemicals Measured in LB in California



```
domain_chem <- chem_measure %>%
  filter(!is.na(Value)) %>%
  group_by(Domain) %>%
  summarise(count = n()) %>%
  arrange(desc(count))
print(domain_chem)
```

Plot above shows the most used chemicals in LB in strawberry harvesting, we can further explore the properties of those chemicals:

```
# Find the index of GHS classification
GHS_searcher<-function(result_json_object){</pre>
  # check if the chemicals in the database first
  if (is.null(result_json_object) ||
      is.null(result_json_object[["result"]]) ||
      is.null(result_json_object[["result"]][["Hierarchies"]]) ||
      is.null(result_json_object[["result"]][["Hierarchies"]][["Hierarchy"]])){
    return("did not find the chemical in the database")
  }
  result<-result_json_object
  for (i in 1:length(result[["result"]][["Hierarchies"]][["Hierarchy"]])){
    if(result[["result"]][["Hierarchies"]][["Hierarchy"]][[i]][["SourceName"]]=="GHS Classificat
      return(i)
    }
}
# Use the output from GHS searcher to access the hazard information
hazards_retriever<-function(index,result_json_object){</pre>
  # Check if GHS_searcher did not find the index
  if (is.character(index) && index == "did not find the chemical in the database") {
    return(index)
  }
  result<-result_json_object
  hierarchy<-result[["result"]][["Hierarchies"]][["Hierarchy"]][[index]]
  output list<-rep(NA,length(hierarchy[["Node"]]))</pre>
  while(str_detect(hierarchy[["Node"]][[i]][["Information"]][["Name"]],"H") & i<length(hierarchy</pre>
[["Node"]])){
    output_list[i]<-hierarchy[["Node"]][[i]][["Information"]][["Name"]]</pre>
    i<-i+1
  return(output_list[!is.na(output_list)])
}
# Find the chemical information for the top chemicals
access_hazard <- function(chemical){</pre>
  results <- list()
  for (chem in chemical){
      result <- get_pug_rest(identifier = chem,
                              namespace = "name",
                              domain = "compound",
                              operation="classification",
                              output = "JSON")
      ghs_index <- GHS_searcher(result)</pre>
      hazards <- hazards_retriever(ghs_index, result)</pre>
      results[[chem]] <- list(
```

```
chem_vec <- top_chem[1:10,]$Chemical_Info</pre>
hazard_info <- access_hazard(chem_vec)</pre>
hazards_df <- do.call(rbind, lapply(hazard_info, function(x) {</pre>
 data.frame(
    chemical_name = x$chemical_name,
    hazards = paste(x$chemical_hazards, collapse = ";"),
    stringsAsFactors = FALSE
  )
}))
hazards_df %>%
 flextable() %>%
 theme_vanilla() %>%
 fontsize(size = 10) %>%
  width(j = "chemical_name", width = 2.5) %>% # Set width for first column
  width(j = "hazards", width = 5) %>% # Set width for second column
  align(align = "left", part = "all") %>%
  set_table_properties(layout = "autofit")
```

chemical_name	hazards
AZADIRACHTIN	NA
TETRACONAZOLE	H302: Harmful if swallowed [Warning Acute toxicity, oral];H300: Health Hazards;Hazard Statement Codes;H302+H332: Harmful if swallowed or if inhaled [Warning Acute toxicity, oral; acute toxicity, inhalation];H332: Harmful if inhaled [Warning Acute toxicity, inhalation];H351: Suspected of causing cancer [Warning Carcinogenicity];H361: Suspected of damaging fertility or the unborn child [Warning Reproductive toxicity];H372: Causes damage to organs through prolonged or repeated exposure [Danger Specific target organ toxicity, repeated exposure];H400: Very toxic to aquatic life [Warning Hazardous to the aquatic environment, acute hazard];H400: Environmental Hazards;H410: Very toxic to aquatic life with long lasting effects [Warning Hazardous to the aquatic environment, long-term hazard]
SPINOSAD	NA

chemical_name	hazards
ABAMECTIN	H260: In contact with water releases flammable gases which may ignite spontaneously [Danger Substances and mixtures which in contact with water, emit flammable gases];H200: Physical Hazards;Hazard Statement Codes;H314: Causes severe skin burns and eye damage [Danger Skin corrosion/irritation];H300: Health Hazards;H317: May cause an allergic skin reaction [Warning Sensitization, Skin];H334: May cause allergy or asthma symptoms or breathing difficulties if inhaled [Danger Sensitization, respiratory];H373: May causes damage to organs through prolonged or repeated exposure [Warning Specific target organ toxicity, repeated exposure]
CYFLUFENAMID	H332: Harmful if inhaled [Warning Acute toxicity, inhalation];H300: Health Hazards;Hazard Statement Codes;H400: Very toxic to aquatic life [Warning Hazardous to the aquatic environment, acute hazard];H400: Environmental Hazards;H410: Very toxic to aquatic life with long lasting effects [Warning Hazardous to the aquatic environment, long-term hazard];H411: Toxic to aquatic life with long lasting effects [Hazardous to the aquatic environment, long-term hazard]
THIAMETHOXAM	NA
CYANTRANILIPROLE	H302: Harmful if swallowed [Warning Acute toxicity, oral];H300: Health Hazards;Hazard Statement Codes;H361: Suspected of damaging fertility or the unborn child [Warning Reproductive toxicity];H371: May cause damage to organs [Warning Specific target organ toxicity, single exposure];H373: May causes damage to organs through prolonged or repeated exposure [Warning Specific target organ toxicity, repeated exposure];H400: Very toxic to aquatic life [Warning Hazardous to the aquatic environment, acute hazard];H400: Environmental Hazards;H410: Very toxic to aquatic life with long lasting effects [Warning Hazardous to the aquatic environment, long-term hazard]
DIFENOCONAZOLE	H302: Harmful if swallowed [Warning Acute toxicity, oral];H300: Health Hazards;Hazard Statement Codes;H302+H332: Harmful if swallowed or if inhaled [Warning Acute toxicity, oral; acute toxicity, inhalation];H319: Causes serious eye irritation [Warning Serious eye damage/eye irritation];H320: Causes eye irritation [Warning Serious eye damage/eye irritation];H332: Harmful if inhaled [Warning Acute toxicity, inhalation];H351: Suspected of causing cancer [Warning Carcinogenicity];H371: May cause damage to organs [Warning Specific target organ toxicity, single exposure];H373: May causes damage to organs through prolonged or repeated exposure [Warning Specific target organ toxicity, repeated exposure];H400: Very toxic to aquatic life [Warning Hazardous to the aquatic environment, acute hazard];H400: Environmental Hazards;H410: Very toxic to aquatic life with long lasting effects [Warning Hazardous to the aquatic environment, long-term hazard]
QUINOLINE	H301: Toxic if swallowed [Danger Acute toxicity, oral];H300: Health Hazards;Hazard Statement Codes;H302: Harmful if swallowed [Warning Acute toxicity, oral];H311: Toxic in contact with skin [Danger Acute toxicity, dermal];H312: Harmful in contact with skin [Warning Acute toxicity, dermal];H315: Causes skin irritation [Warning Skin corrosion/irritation];H319: Causes serious eye irritation [Warning Serious eye damage/eye irritation];H335: May cause respiratory irritation [Warning Specific target organ toxicity, single exposure; Respiratory tract irritation];H336: May cause drowsiness or dizziness [Warning Specific target organ toxicity, single exposure; Narcotic effects];H341: Suspected of causing genetic defects [Warning Germ cell mutagenicity];H350: May cause cancer [Danger Carcinogenicity];H351: Suspected of causing cancer [Warning Carcinogenicity];H370: Causes damage to organs [Danger Specific target organ toxicity, single exposure];H371: May cause damage to organs [Warning Specific target organ toxicity, single exposure];H373: May cause damage to organs through prolonged or repeated exposure [Warning Specific target organ toxicity, repeated exposure];H400: Very toxic to aquatic life [Warning Hazardous to the aquatic environment, acute hazard];H400: Environmental Hazards;H402: Harmful to aquatic life [Hazardous to the aquatic environment, acute hazard];H410: Very toxic to aquatic life with long lasting effects [Warning Hazardous to the aquatic environment, long-term hazard];H411: Toxic to aquatic life with long lasting effects [Hazardous to the aquatic environment, long-term hazard];H412:

chemical_name	hazards
	Harmful to aquatic life with long lasting effects [Hazardous to the aquatic environment, long-term hazard]
HEXYTHIAZOX	H320: Causes eye irritation [Warning Serious eye damage/eye irritation];H300: Health Hazards;Hazard Statement Codes;H400: Very toxic to aquatic life [Warning Hazardous to the aquatic environment, acute hazard];H400: Environmental Hazards;H410: Very toxic to aquatic life with long lasting effects [Warning Hazardous to the aquatic environment, long-term hazard];Hazardous to the aquatic environment, acute hazard;Environmental Hazards;Hazard Classes;Hazardous to the aquatic environment, long-term hazard

Through the chemical information presented in the above table, seven out of the top ten chemicals have hazards information. Especially for QUINOLINE, which can cause damage to organs and toxic in contact. Also, most of those chemicals are very toxic to aquatic life, which will harm the sustainable development of the environment. Additionally, most of the top used chemicals belong to insecticide group, and this suggests that many of the chemicals used in California are used for pest control. This phenomenon could be the result of large production of strawberry and warm weather in California.

Now, we can further analyze the top chemicals used in strawberry growing in Florida:

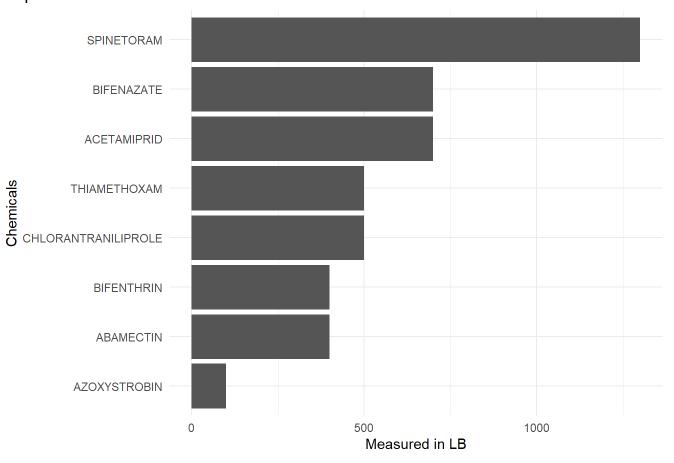
```
# Select records with Florida only chemicals
df_measure_lb <- df_flo %>%
  filter(Measurement=="MEASURED IN LB") %>%
  filter(!is.na(Value)) %>%
  filter(Chemical_Info != "TOTAL")

print(unique(df_measure_lb$Chemical_Info))
```

```
## [1] "AZOXYSTROBIN" "ABAMECTIN" "ACETAMIPRID"
## [4] "BIFENTHRIN" "CHLORANTRANILIPROLE" "THIAMETHOXAM"
## [7] "SPINETORAM" "BIFENAZATE"
```

Ignoring "Total" variable, here are the eight chemicals that are used most in Florida when measurement in LB.

Top Chemicals Used in Florida



```
chem_vec_flo <- top_chem$Chemical_Info</pre>
hazard_info_flo <- access_hazard(chem_vec_flo)</pre>
hazards_df_flo <- do.call(rbind, lapply(hazard_info_flo, function(x) {</pre>
  data.frame(
    chemical_name = x$chemical_name,
    hazards = paste(x$chemical_hazards, collapse = ";"),
    stringsAsFactors = FALSE
  )
}))
hazards_df_flo %>%
 flextable() %>%
 theme_vanilla() %>%
  fontsize(size = 10) %>%
  width(j = "chemical_name", width = 2.5) %>% # Set width for first column
  width(j = "hazards", width = 5) %>% # Set width for second column
  align(align = "left", part = "all") %>%
  set_table_properties(layout = "autofit")
```

chemical_name	hazards
SPINETORAM	NA
ACETAMIPRID	H301: Toxic if swallowed [Danger Acute toxicity, oral];H300: Health Hazards;Hazard Statement Codes;H302: Harmful if swallowed [Warning Acute toxicity, oral];H330: Fatal if

chemical_name	hazards
	inhaled [Danger Acute toxicity, inhalation];H332: Harmful if inhaled [Warning Acute toxicity, inhalation];H351: Suspected of causing cancer [Warning Carcinogenicity];H361d: Suspected of damaging the unborn child [Warning Reproductive toxicity];H370: Causes damage to organs [Danger Specific target organ toxicity, single exposure];H371: May cause damage to organs [Warning Specific target organ toxicity, single exposure];H373: May causes damage to organs through prolonged or repeated exposure [Warning Specific target organ toxicity, repeated exposure];H400: Very toxic to aquatic life [Warning Hazardous to the aquatic environment, acute hazard];H400: Environmental Hazards;H402: Harmful to aquatic life [Hazardous to the aquatic environment, acute hazard];H410: Very toxic to aquatic life with long lasting effects [Warning Hazardous to the aquatic environment, long-term hazard];H411: Toxic to aquatic life with long lasting effects [Hazardous to the aquatic environment, long-term hazard];H412: Harmful to aquatic life with long lasting effects [Hazardous to the aquatic environment, long-term hazard]
BIFENAZATE	H317: May cause an allergic skin reaction [Warning Sensitization, Skin];H300: Health Hazards;Hazard Statement Codes;H319: Causes serious eye irritation [Warning Serious eye damage/eye irritation];H320: Causes eye irritation [Warning Serious eye damage/eye irritation];H372: Causes damage to organs through prolonged or repeated exposure [Danger Specific target organ toxicity, repeated exposure];H373: May causes damage to organs through prolonged or repeated exposure [Warning Specific target organ toxicity, repeated exposure];H400: Very toxic to aquatic life [Warning Hazardous to the aquatic environment, acute hazard];H400: Environmental Hazards;H410: Very toxic to aquatic life with long lasting effects [Warning Hazardous to the aquatic environment, long-term hazard];Hazardous to the aquatic environment, long-term hazard
CHLORANTRANILIPROLE	H319: Causes serious eye irritation [Warning Serious eye damage/eye irritation];H300: Health Hazards;Hazard Statement Codes;H335: May cause respiratory irritation [Warning Specific target organ toxicity, single exposure; Respiratory tract irritation];H336: May cause drowsiness or dizziness [Warning Specific target organ toxicity, single exposure; Narcotic effects];H351: Suspected of causing cancer [Warning Carcinogenicity];H360: May damage fertility or the unborn child [Danger Reproductive toxicity];H373: May causes damage to organs through prolonged or repeated exposure [Warning Specific target organ toxicity, repeated exposure];H400: Very toxic to aquatic life [Warning Hazardous to the aquatic environment, acute hazard];H400: Environmental Hazards;H401: Toxic to aquatic life [Hazardous to the aquatic environment, acute hazard];H410: Very toxic to aquatic life with long lasting effects [Warning Hazardous to the aquatic environment, long-term hazard]
THIAMETHOXAM	NA
ABAMECTIN	H260: In contact with water releases flammable gases which may ignite spontaneously [Danger Substances and mixtures which in contact with water, emit flammable gases];H200: Physical Hazards;Hazard Statement Codes;H314: Causes severe skin burns and eye damage [Danger Skin corrosion/irritation];H300: Health Hazards;H317: May cause an allergic skin reaction [Warning Sensitization, Skin];H334: May cause allergy or asthma symptoms or breathing difficulties if inhaled [Danger Sensitization, respiratory];H373: May causes damage to organs through prolonged or repeated exposure [Warning Specific target organ toxicity, repeated exposure]
BIFENTHRIN	NA
AZOXYSTROBIN	H331: Toxic if inhaled [Danger Acute toxicity, inhalation];H300: Health Hazards;Hazard Statement Codes;H370: Causes damage to organs [Danger Specific target organ toxicity, single exposure];H400: Very toxic to aquatic life [Warning Hazardous to the aquatic environment, acute hazard];H400: Environmental Hazards;H410: Very toxic to

chemical_name	hazards
	aquatic life with long lasting effects [Warning Hazardous to the aquatic environment, long-term hazard]

Through the table shown above, five out of top eight chemicals used in Florida have hazard information. The most toxic chemical is the azoxystrobin, which can be toxic if inhaled, and it also causes damage to organs with single exposure. Additionally, it has toxic effects to aquatic lives, which is bad for the environment. Also, 7 out of top 8 chemicals used are insecticide, this may relate to the location of Florida, which is already in the tropical area. The warmer weather brings more insects, so the farmers there need to use more insecticide for pest control. The principal pests on strawberry in Florida are the twospotted spider mite and lepidopterous larvae.

In summary, by comparing the chemicals used in California and Florida, California used more types of chemicals than Florida, also, the counts of chemicals used in growing strawberry were also higher for California, which is almost two times of Florida's value. However, California and Florida both used chemicals in insecticide that are toxic to the aquatic lives, environment and human's health, and it is important to suggest to the government to restrict the amount of harmful chemicals used in insecticides and pesticides, and they should be changed to more environmental friendly substitutes.