# NMF Final (Only nndsvd 5 component without ozone)

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```
# load the packages
library(NMF)
library(tidyverse)
library(gridExtra)
library(readxl)
library(circular)
library(lwgeom)
library(units)
```

## Procedure

1. Remove hourly observation with missing observation for any chemical
2. Remove background noise level using min values (except for chemicals with minimum value < 2*LOD and maximum value > 100*LOD)
3. Zero values are converted to a random value between 0 and 0.5*LOD
4. Normalize using min and max
5. Remove Ozone (wouldn't affect # of obs.)

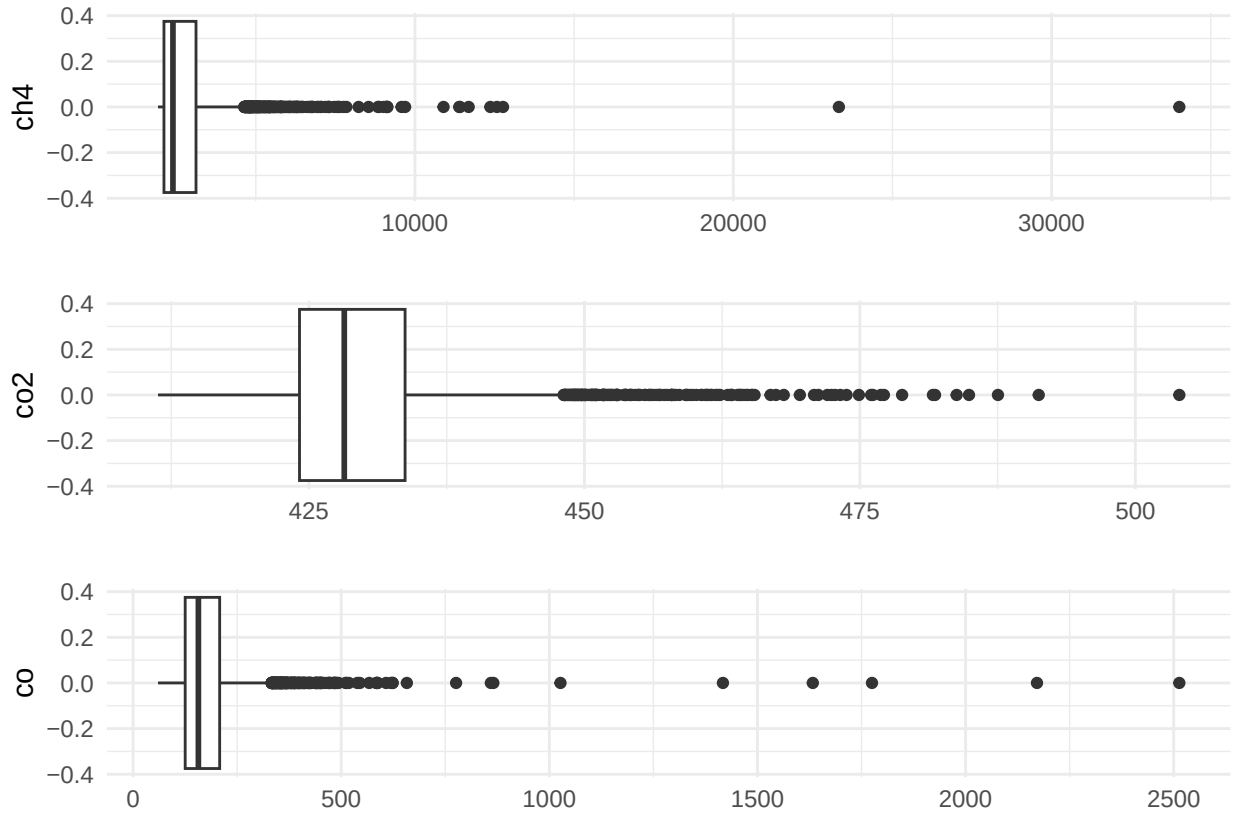
### Reading the data

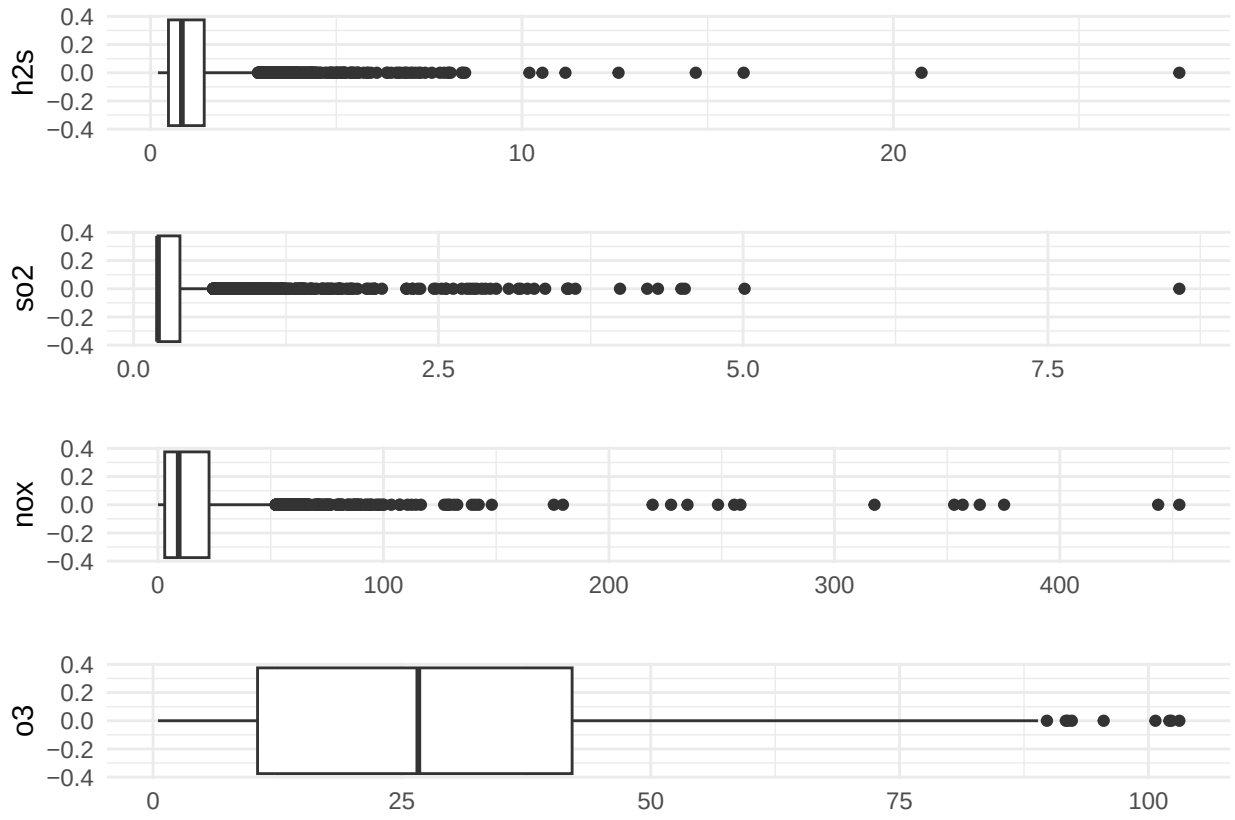
```
hourly_data <- readRDS("../DataProcessing/Trailer_hourly_merge_20240905.rds")
```

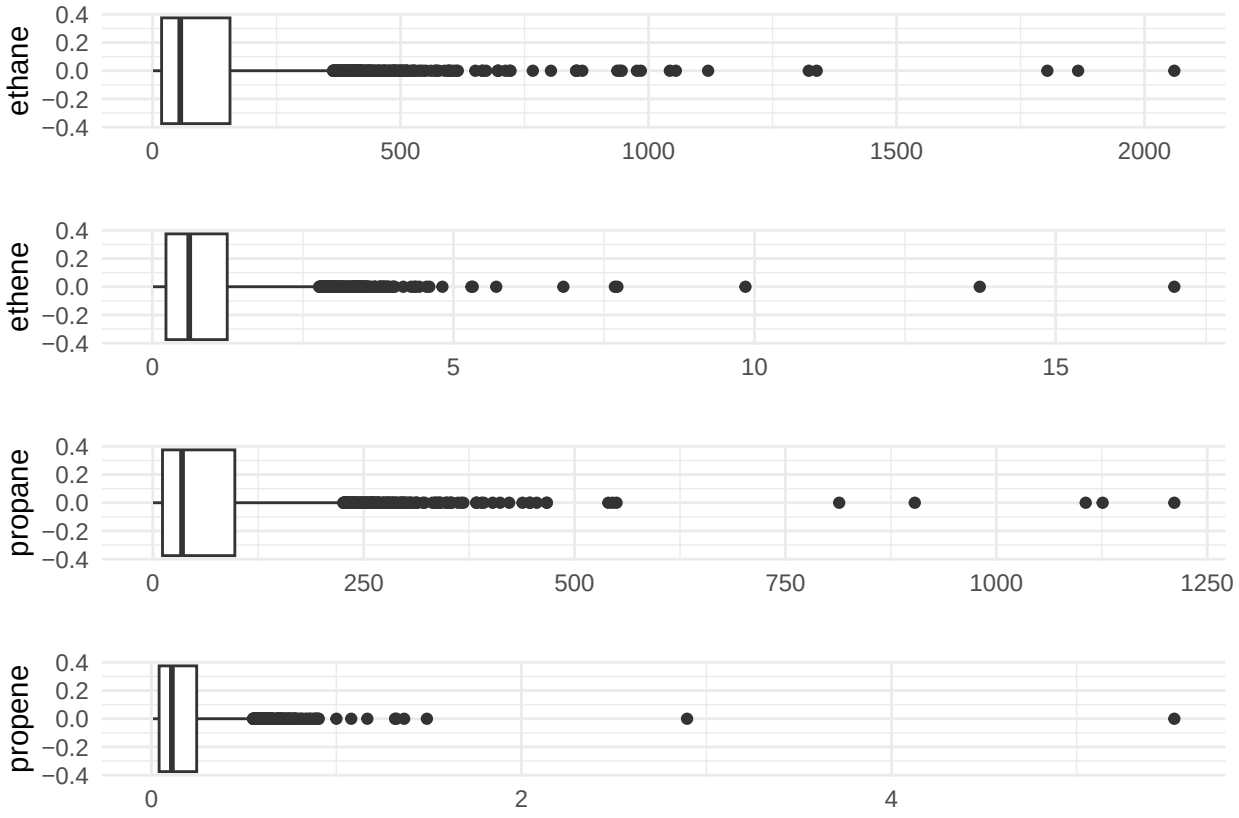
```
# PROCEDURE STEP 1:
hourly_data <- hourly_data %>% rename('co2' = 'co2_ppm')

vocs <- c("ethane", "ethene", "propane", "propene",
                                        "1_3-butadiene", "i-butane", "n-butane",
                                        "acetylene", "cyclopentane", "i-pentane",
                                        "n-pentane", "n-hexane", "isoprene", "n-heptane",
                                        "benzene", "n-octane", "toluene", "ethyl-benzene",
                                        "m&p-xylene", "o-xylene")


non_vocs <- c('ch4', 'co2', 'co', 'h2s', 'so2', 'nox', 'o3')

# remove row with missing obs for any chemical
hourly_nona <- hourly_data %>%
```

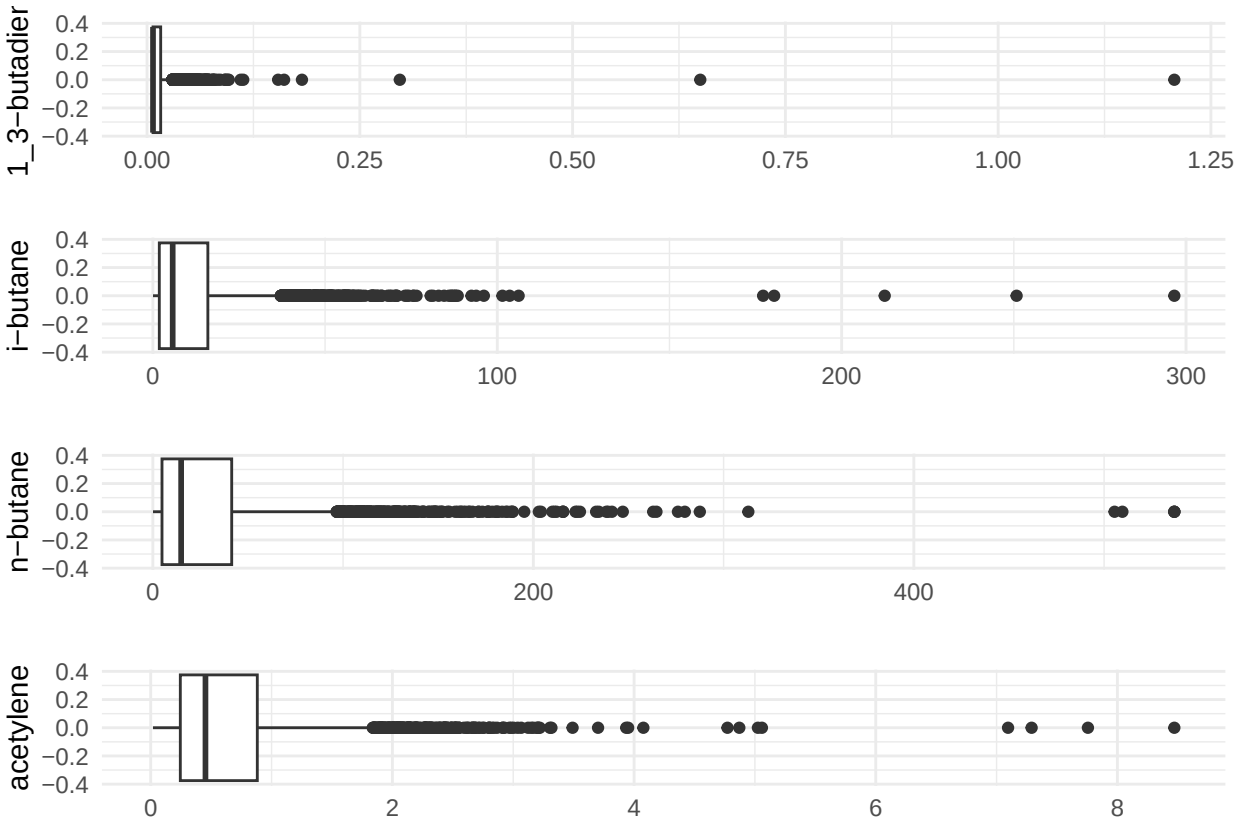
```
  select(any_of(c('day', 'time_utc', vocs, non_vocs, 'wdr_deg', 'wsp_ms'))) %>%
  na.omit()

# retrieving the vocs, removing everything else except the vocs
hourly_vocs <- hourly_nona %>% select(any_of(vocs))

# retrieving the non-vocs: co2_ppm, nox, ch4, h2s, so2, o3
# double check this
hourly_non_vocs <- hourly_nona %>% select(any_of(non_vocs))

hourly_full_nona <- cbind(hourly_non_vocs, hourly_vocs)

# retrive a vector of yearmonth
hourly_dates <- hourly_nona %>%
  mutate(yearmonth = substring(day, 0, 7)) %>%
  pull(yearmonth)
```

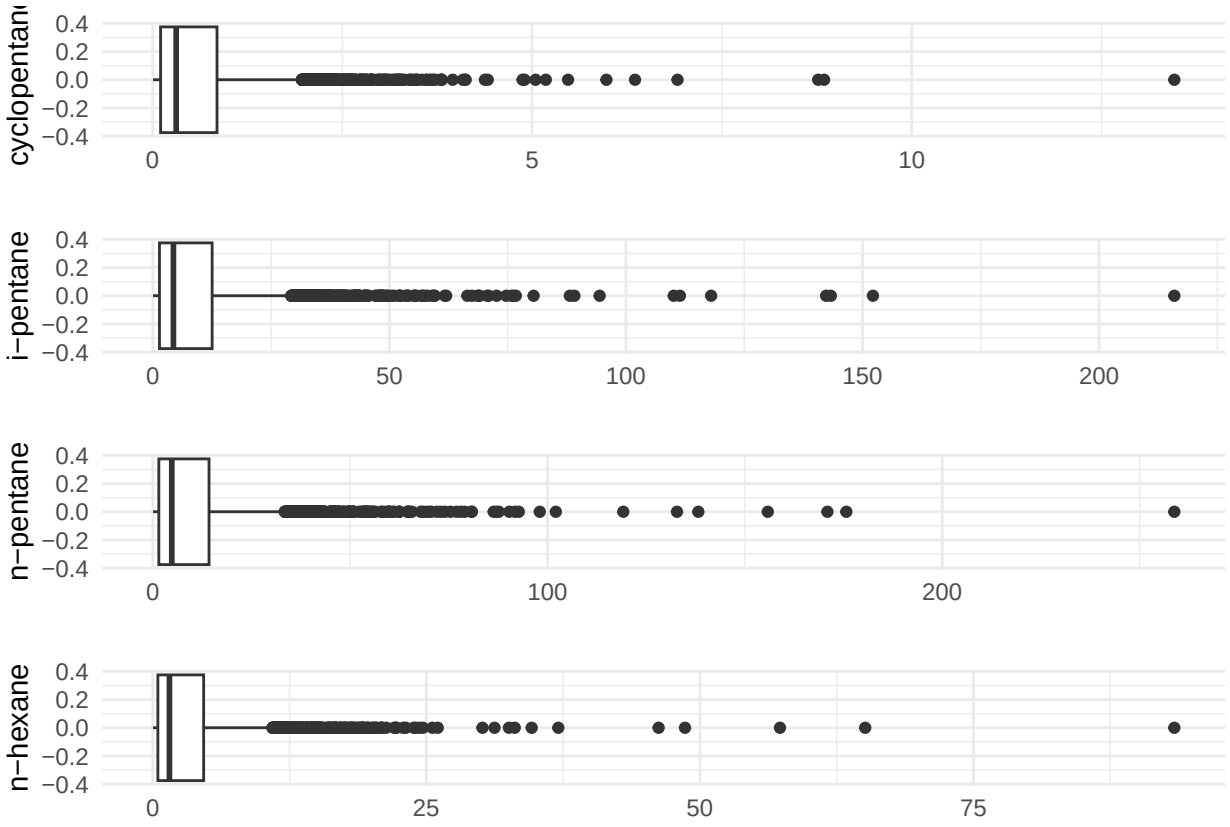
## Data visualisation

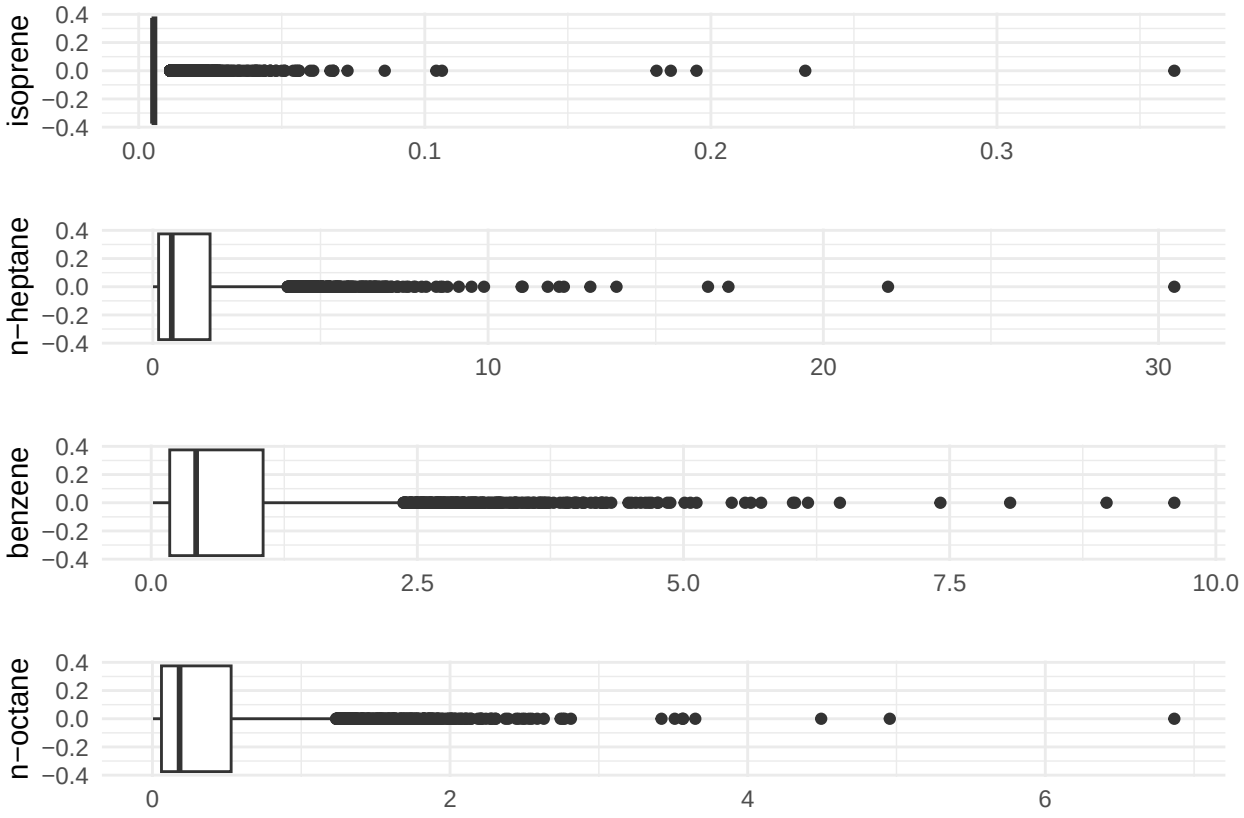


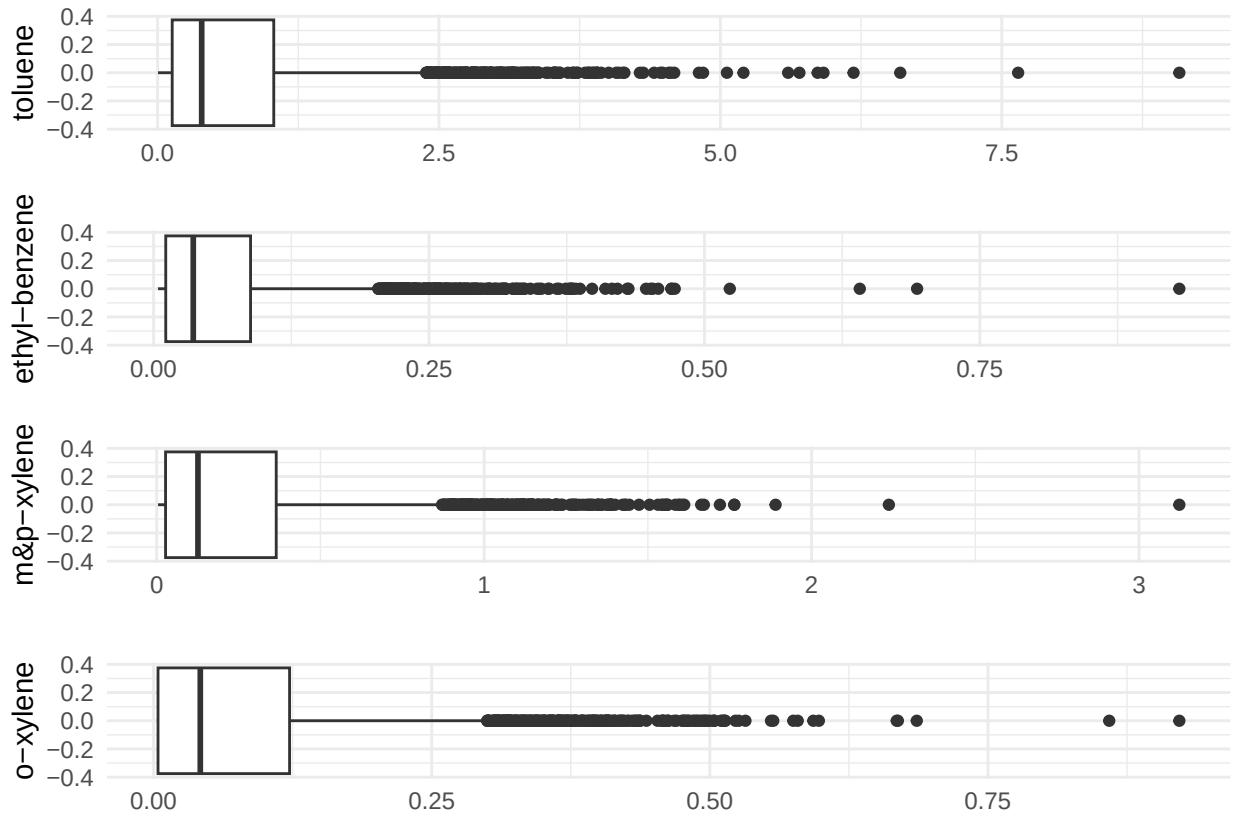

h2s
0.4
0.2
0.0
−0.2
−0.4
0
10
20
so2
0.4
0.2
0.0
−0.2
−0.4
0.0
2.5
5.0
7.5
nox
0.4
0.2
0.0
−0.2
−0.4
0
100
200
300
400
o3
0.4
0.2
0.0
−0.2
−0.4
0
25
50
75
100


ethane
0.4
0.2
0.0
−0.2
−0.4
0
500
1000
1500
2000
ethene
0.4
0.2
0.0
−0.2
−0.4
0
5
10
15
propane
0.4
0.2
0.0
−0.2
−0.4
0
250
500
750
1000
1250
propene
0.4
0.2
0.0
−0.2
−0.4
0
2
4


1_3−butadier
0.4
0.2
0.0
−0.2
−0.4
0.00
0.25
0.50
0.75
1.00
1.25
i−butane
0
100
200
300
n−butane
0
200
400
acetylene
0
2
4
6
8


cyclopentan
i−pentane
n−pentane
n−hexane
0.4
0.2
0.0
−0.2
−0.4
0
5
10
50
100
150
200
25
75


isoprene
0.4
0.2
0.0
−0.2
−0.4
0.0
0.1
0.2
0.3
n−heptane
0
10
20
30
benzene
0.0
2.5
5.0
7.5
10.0
n−octane
0
2
4
6




**Data preprocessing**

```
# Define LOD for each chemical
LOD_non_voc <- c('ch4' = 0.9,
                 'co2' = 0.0433,
                 'co' = 40,
                 'h2s' = 0.4,
                 'so2' = 0.4,
                 'nox' = 0.05,
                 'o3' = 1)

# LOD_voc_monthly <- read_csv('../data/LNM_VOC_LOD_Rounded.csv') %>% select(-1)
#
# # extract the yearmonth from date variables
# LOD_voc_monthly <- LOD_voc_monthly %>%
#   mutate(yearmonth = strftime(as.POSIXct(start_date, format = '%Y-%m-%d %H:%M:%S', tz = 'UTC'), '%Y-%
#
# LOD_voc_monthly <- LOD_voc_monthly %>%
#   select(-c(start_date, end_date)) %>%
#   select(!any_of(ends_with('half_ldl')))
#
# colnames(LOD_voc_monthly) <- str_replace_all(names(LOD_voc_monthly), '_ldl', '')

LOD_voc_avg <- read_xlsx('../data/LNM_VOC_Uncertainties.xlsx', skip = 1)
```

```
LOD_voc_avg <- LOD_voc_avg %>%
  select(1, 4) %>%
  rename('LOD' = 2, 'chemical' = 1) %>%
  head(20)
```

```
# find the min for background-levels
background_levels <- sapply(hourly_full_nona, min)
background_levels
```

```
##           ch4           co2            co           h2s           so2
##      1928.000       411.300        59.910         0.200         0.200
##           nox            o3        ethane        ethene       propane
##         0.025         0.500         0.916         0.011         0.224
##       propene 1_3-butadiene      i-butane      n-butane     acetylene
##         0.009         0.007         0.035         0.090         0.019
##  cyclopentane     i-pentane     n-pentane      n-hexane      isoprene
##         0.005         0.038         0.042         0.021         0.005
##     n-heptane       benzene      n-octane       toluene ethyl-benzene
##         0.004         0.017         0.004         0.004         0.004
##    m&p-xylene      o-xylene
##         0.004         0.004
```

```
# Show a table of summary statistics
get_info <- function(column) {
  N <- length(column)
  background <- quantile(column, 0)
  quantile1 <- quantile(column, 0.01)
  quantile99 <- quantile(column, 0.99)
  n_background <- sum(column == background)
  max <- max(column)
  return(c(N, quantile1, quantile99, max, background, n_background))
}

info_table <- hourly_full_nona %>%
  reframe(across(everything(), ~ get_info(.x)))

info_table <- info_table %>%
  mutate(rownames = c('N', '1st percentile', '99th percentile', 'Max', 'Background', '# Background')) %
  pivot_longer(-rownames) %>%
  pivot_wider(names_from = rownames, values_from = value)

knitr::kable(info_table)
```

| name | N | 1st percentile | 99th percentile | Max | Background | # Background |
|---|---|---|---|---|---|---|
| ch4 | 4788 | 1962.98700 | 6286.12400 | 34010.900 | 1928.000 | 1 |
| co2 | 4788 | 416.47870 | 460.62260 | 503.990 | 411.300 | 1 |
| co | 4788 | 84.23050 | 442.08860 | 2513.440 | 59.910 | 1 |
| h2s | 4788 | 0.20000 | 5.20986 | 27.700 | 0.200 | 829 |
| so2 | 4788 | 0.20000 | 1.78686 | 8.578 | 0.200 | 3266 |
| nox | 4788 | 0.22974 | 89.72371 | 452.959 | 0.025 | 2 |

| name | N | 1st percentile | 99th percentile | Max | Background | # Background |
|---|---|---|---|---|---|---|
| o3 | 4788 | 0.50000 | 76.02600 | 103.100 | 0.500 | 259 |
| ethane | 4788 | 1.84422 | 526.44700 | 2060.000 | 0.916 | 1 |
| ethene | 4788 | 0.01100 | 3.50826 | 16.970 | 0.011 | 163 |
| propane | 4788 | 0.84674 | 300.79000 | 1211.000 | 0.224 | 1 |
| propene | 4788 | 0.00900 | 0.69739 | 5.528 | 0.009 | 411 |
| 1_3-butadiene | 4788 | 0.00700 | 0.05900 | 1.207 | 0.007 | 3357 |
| i-butane | 4788 | 0.15148 | 60.89400 | 296.600 | 0.035 | 1 |
| n-butane | 4788 | 0.37248 | 166.52100 | 536.900 | 0.090 | 1 |
| acetylene | 4788 | 0.04900 | 2.61304 | 8.471 | 0.019 | 2 |
| cyclopentane | 4788 | 0.00500 | 3.06899 | 13.460 | 0.005 | 96 |
| i-pentane | 4788 | 0.10987 | 49.60210 | 215.900 | 0.038 | 1 |
| n-pentane | 4788 | 0.10487 | 55.95980 | 258.800 | 0.042 | 1 |
| n-hexane | 4788 | 0.04300 | 18.17780 | 93.360 | 0.021 | 2 |
| isoprene | 4788 | 0.00500 | 0.03313 | 0.362 | 0.005 | 2816 |
| n-heptane | 4788 | 0.01500 | 6.57669 | 30.470 | 0.004 | 5 |
| benzene | 4788 | 0.02800 | 3.78693 | 9.610 | 0.017 | 3 |
| n-octane | 4788 | 0.00400 | 2.00839 | 6.867 | 0.004 | 100 |
| toluene | 4788 | 0.01300 | 3.52165 | 9.077 | 0.004 | 11 |
| ethyl-benzene | 4788 | 0.00400 | 0.31613 | 0.931 | 0.004 | 918 |
| m&p-xylene | 4788 | 0.00400 | 1.29156 | 3.123 | 0.004 | 851 |
| o-xylene | 4788 | 0.00400 | 0.45700 | 0.922 | 0.004 | 1330 |

```
# PROCEDURE STEP 2:
#adjustments that were made according to paper
#William: I'm guessing this refers to Gunnar's paper section 2.2 and Guha 3.3

# Check whether chemical has background noise level that needs to be removed
# i.e, NO ADJUSTMENT if minimum value < 2*LOD and maximum value > 100*LOD
adjusting_neg_bg_from_lod <- function(chemical, LOD, background, hourly_data){
    # get min and max
    min_value <- min(hourly_data[chemical], na.rm = TRUE)
    max_value <- max(hourly_data[chemical], na.rm = TRUE)
    # if min less than double LOD or max > 100 times LOD
    # adjust to -100 (for entire column???)
    if (min_value < 2 * LOD & max_value > 100 * LOD ){
      return (0)
    }
  return (background)
}
```

```
# Check if background is negligible for non voc
# merge background and LOD
background_lod_non_voc <- tibble(chemical = non_vocs,
                                 LOD = LOD_non_voc,
                                 background = unname(background_levels[non_vocs]))
adjusted_background_non_voc <- background_lod_non_voc %>%
  rowwise() %>%
  mutate(min = min(hourly_full_nona[chemical], na.rm = TRUE),
         LODx2 = 2 * LOD,
         criterion1 = min(hourly_full_nona[chemical], na.rm = TRUE) < 2 * LOD,
         max = max(hourly_full_nona[chemical], na.rm = TRUE),
```

```
         LODx100 = 100 * LOD,
         criterion2 = max(hourly_full_nona[chemical], na.rm = TRUE) > 100 * LOD,
         adjusted_background = adjusting_neg_bg_from_lod(chemical, LOD, background, hourly_full_nona))
```

```
# Check if background is negligible for voc
# merge background and LOD
background_lod_voc <- LOD_voc_avg %>%
  left_join(tibble(chemical = setdiff(names(background_levels), non_vocs),
                   background = background_levels[setdiff(names(background_levels), non_vocs)]))
```

```
## Joining with `by = join_by(chemical)`
```

```
adjusted_background_voc <- background_lod_voc %>%
  rowwise() %>%
  mutate(min = min(hourly_full_nona[chemical], na.rm = TRUE),
         LODx2 = 2 * LOD,
         criterion1 = min(hourly_full_nona[chemical], na.rm = TRUE) < 2 * LOD,
         max = max(hourly_full_nona[chemical], na.rm = TRUE),
         LODx100 = 100 * LOD,
         criterion2 = max(hourly_full_nona[chemical], na.rm = TRUE) > 100 * LOD,
         adjusted_background = adjusting_neg_bg_from_lod(chemical, LOD, background, hourly_full_nona))
```

```
# So now we have the adjusted background concentrations
hourly_nona_bgrm <- hourly_full_nona %>%
  mutate(across(adjusted_background_non_voc$chemical, ~  .x - adjusted_background_non_voc$adjusted_backg
hourly_nona_bgrm <- hourly_nona_bgrm %>%
  mutate(across(adjusted_background_voc$chemical, ~  .x - adjusted_background_voc$adjusted_background[ac
```

```
# look at zero values
colSums(hourly_nona_bgrm == 0)
```

```
##           ch4           co2            co           h2s           so2
##             1             1             1           829          3266
##           nox            o3        ethane        ethene       propane
##             0             0             1             0             1
##       propene 1_3-butadiene      i-butane      n-butane     acetylene
##             0          3357             1             1             0
##  cyclopentane     i-pentane     n-pentane      n-hexane      isoprene
##             0             1             1             2          2816
##     n-heptane       benzene      n-octane       toluene ethyl-benzene
##             0             0             0             0             0
##    m&p-xylene      o-xylene
##             0             0
```

```
# PROCEDURE STEP 3
# replace zero values with random values between 0 and 0.5*LOD
set.seed(123)
replace_zero_with_random <- function(column, name, LOD_df){
  LOD <- LOD_df$LOD[LOD_df$chemical == name]
  column <- if_else(column == 0, round(runif(length(column), 0, 0.5 * LOD), 3), column)
  return (column)
```

```
}

hourly_nona_bgrm_zerorepl <- hourly_nona_bgrm %>%
  mutate(across(adjusted_background_non_voc$chemical, ~ replace_zero_with_random(.x, cur_column(), adju

hourly_nona_bgrm_zerorepl <- hourly_nona_bgrm_zerorepl %>%
  mutate(across(adjusted_background_voc$chemical, ~ replace_zero_with_random(.x, cur_column(), adjusted_
```

### Normalize the non-vocs

```
#normalizing function
normalize_column <- function(column){
  background <- quantile(column, 0)
  max <- quantile(column, 1) # this could be adjusted
  return ((column - background)/(max - background))
}
```

```
# normalize all
hourly_nona_bgrm_zerorepl_norm <- as_tibble(sapply(as.list(hourly_nona_bgrm_zerorepl), normalize_column
summary(hourly_nona_bgrm_zerorepl_norm)
```

```
##       ch4                co2               co                h2s
##  Min.   :0.000000   Min.   :0.0000   Min.   :0.00000   Min.   :0.00000
##  1st Qu.:0.005795   1st Qu.:0.1384   1st Qu.:0.02592   1st Qu.:0.01022
##  Median :0.014603   Median :0.1823   Median :0.03884   Median :0.02335
##  Mean   :0.026837   Mean   :0.2000   Mean   :0.04761   Mean   :0.03500
##  3rd Qu.:0.037200   3rd Qu.:0.2418   3rd Qu.:0.05970   3rd Qu.:0.04525
##  Max.   :1.000000   Max.   :1.0000   Max.   :1.00000   Max.   :1.00000
##       so2                nox                o3              ethane
##  Min.   :0.000000   Min.   :0.000000   Min.   :0.00000   Min.   :0.000000
##  1st Qu.:0.007997   1st Qu.:0.006534   1st Qu.:0.09747   1st Qu.:0.008386
##  Median :0.016114   Median :0.020262   Median :0.25487   Median :0.026672
##  Mean   :0.026320   Mean   :0.036440   Mean   :0.26676   Mean   :0.050993
##  3rd Qu.:0.023633   3rd Qu.:0.049978   3rd Qu.:0.40546   3rd Qu.:0.075376
##  Max.   :1.000000   Max.   :1.000000   Max.   :1.00000   Max.   :1.000000
##      ethene            propane            propene          1_3-butadiene
##  Min.   :0.00000   Min.   :0.000000   Min.   :0.000000   Min.   :0.000000
##  1st Qu.:0.01268   1st Qu.:0.009285   1st Qu.:0.005979   1st Qu.:0.001667
##  Median :0.03547   Median :0.028411   Median :0.018482   Median :0.004167
##  Mean   :0.05042   Mean   :0.053805   Mean   :0.028772   Mean   :0.007368
##  3rd Qu.:0.07266   3rd Qu.:0.080132   3rd Qu.:0.042761   3rd Qu.:0.007500
##  Max.   :1.00000   Max.   :1.000000   Max.   :1.000000   Max.   :1.000000
##     i-butane           n-butane          acetylene        cyclopentane
##  Min.   :0.000000   Min.   :0.000000   Min.   :0.00000   Min.   :0.000000
##  1st Qu.:0.006153   1st Qu.:0.008783   1st Qu.:0.02674   1st Qu.:0.007432
##  Median :0.019261   Median :0.027528   Median :0.05135   Median :0.022668
##  Mean   :0.038384   Mean   :0.054906   Mean   :0.07436   Mean   :0.043730
##  3rd Qu.:0.053703   3rd Qu.:0.077047   3rd Qu.:0.10211   3rd Qu.:0.062653
##  Max.   :1.000000   Max.   :1.000000   Max.   :1.00000   Max.   :1.000000
##    i-pentane          n-pentane          n-hexane           isoprene
##  Min.   :0.000000   Min.   :0.000000   Min.   :0.000000   Min.   :0.000000
```

```
##  1st Qu.:0.006293   1st Qu.:0.005681   1st Qu.:0.004725   1st Qu.:0.002801
##  Median :0.019932   Median :0.018371   Median :0.016060   Median :0.005602
##  Mean   :0.041085   Mean   :0.038859   Mean   :0.035000   Mean   :0.010304
##  3rd Qu.:0.057848   3rd Qu.:0.054837   3rd Qu.:0.049564   3rd Qu.:0.011204
##  Max.   :1.000000   Max.   :1.000000   Max.   :1.000000   Max.   :1.000000
##    n-heptane          benzene           n-octane           toluene
##  Min.   :0.000000   Min.   :0.00000   Min.   :0.000000   Min.   :0.00000
##  1st Qu.:0.005473   1st Qu.:0.01637   1st Qu.:0.008269   1st Qu.:0.01389
##  Median :0.018348   Median :0.04222   Median :0.026009   Median :0.04276
##  Mean   :0.039328   Mean   :0.07655   Mean   :0.054341   Mean   :0.07825
##  3rd Qu.:0.055866   3rd Qu.:0.10779   3rd Qu.:0.076497   3rd Qu.:0.11333
##  Max.   :1.000000   Max.   :1.00000   Max.   :1.000000   Max.   :1.00000
##  ethyl-benzene        m&p-xylene          o-xylene
##  Min.   :0.000000   Min.   :0.000000   Min.   :0.00000
##  1st Qu.:0.007551   1st Qu.:0.007374   1st Qu.:0.00000
##  Median :0.034520   Median :0.039115   Median :0.04139
##  Mean   :0.062378   Mean   :0.077508   Mean   :0.08650
##  3rd Qu.:0.090615   3rd Qu.:0.115742   3rd Qu.:0.12881
##  Max.   :1.000000   Max.   :1.000000   Max.   :1.00000
```

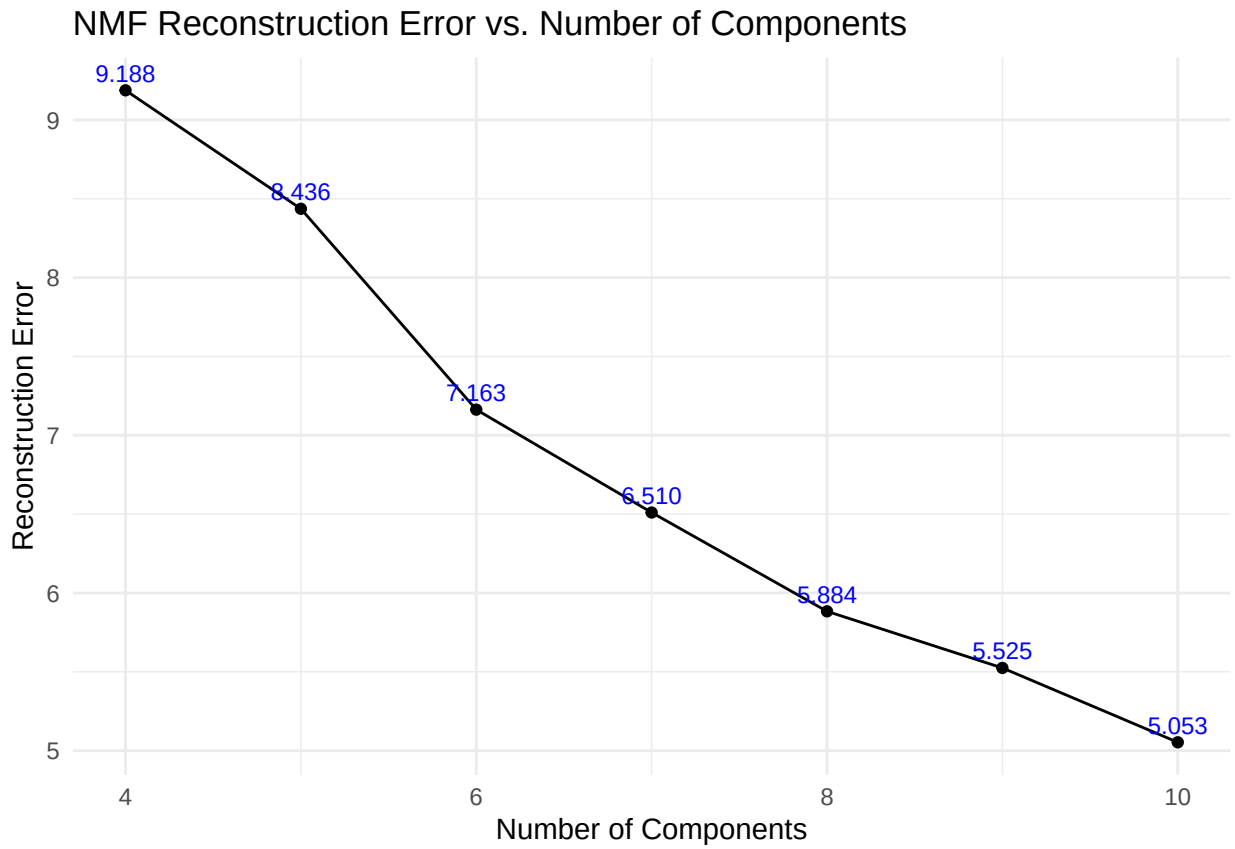
```
normalized_matrix <- as.matrix(hourly_nona_bgrm_zerorepl_norm) #important: using the normalized VOCs fo
```

## NMF section

### Helper for source contributions plots

### NMF using 'nndsvd' seed and KL divergence

```
components <- 4:10
errors <- numeric(length(components) - 4)

# Loop over the number of components
# for (n in components) {
#   nmf_result <- nmf(normalized_matrix, rank = n, method = "KL", seed='nndsvd')
#   reconstruction <- basis(nmf_result) %*% coef(nmf_result)
#   error <- norm(normalized_matrix - reconstruction, type = "F")
#   errors[n-3] <- error
#   print(paste0('Completed ', n - 3, ' out of 7'))
# }
#
# saveRDS(errors, 'errors_norm.rds')

errors <- readRDS('errors_norm.rds')
```



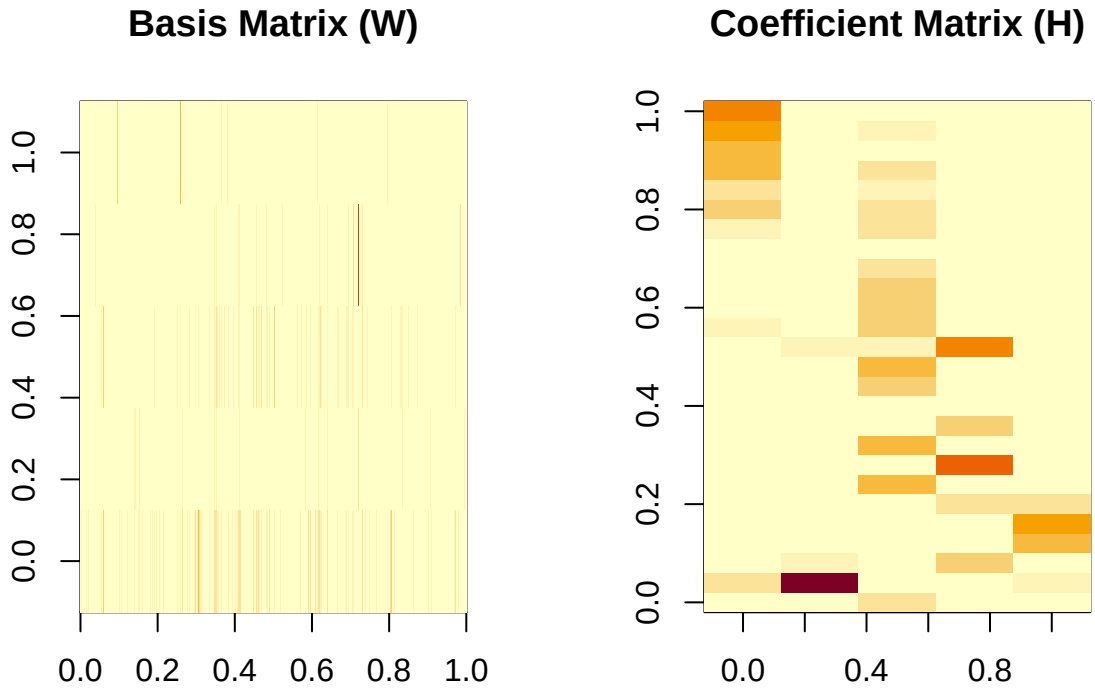

## 5 Components without ozone

```
normalized_matrix_less_o3 <- normalized_matrix[ ,setdiff(colnames(normalized_matrix), "o3")]

nmf_result_5c_less_o3 <- nmf(normalized_matrix_less_o3, rank = 5, method = "KL", seed='nndsvd')
```

```
## Warning in sqrt(S[i] * termn) * uun: Recycling array of length 1 in array-vector arithmetic is depre
##   Use c() or as.vector() instead.

## Warning in sqrt(S[i] * termn) * vvn: Recycling array of length 1 in array-vector arithmetic is depre
##   Use c() or as.vector() instead.

## Warning in sqrt(S[i] * termn) * uun: Recycling array of length 1 in array-vector arithmetic is depre
##   Use c() or as.vector() instead.

## Warning in sqrt(S[i] * termn) * vvn: Recycling array of length 1 in array-vector arithmetic is depre
##   Use c() or as.vector() instead.

## Warning in sqrt(S[i] * termn) * uun: Recycling array of length 1 in array-vector arithmetic is depre
##   Use c() or as.vector() instead.

## Warning in sqrt(S[i] * termn) * vvn: Recycling array of length 1 in array-vector arithmetic is depre
##   Use c() or as.vector() instead.
```

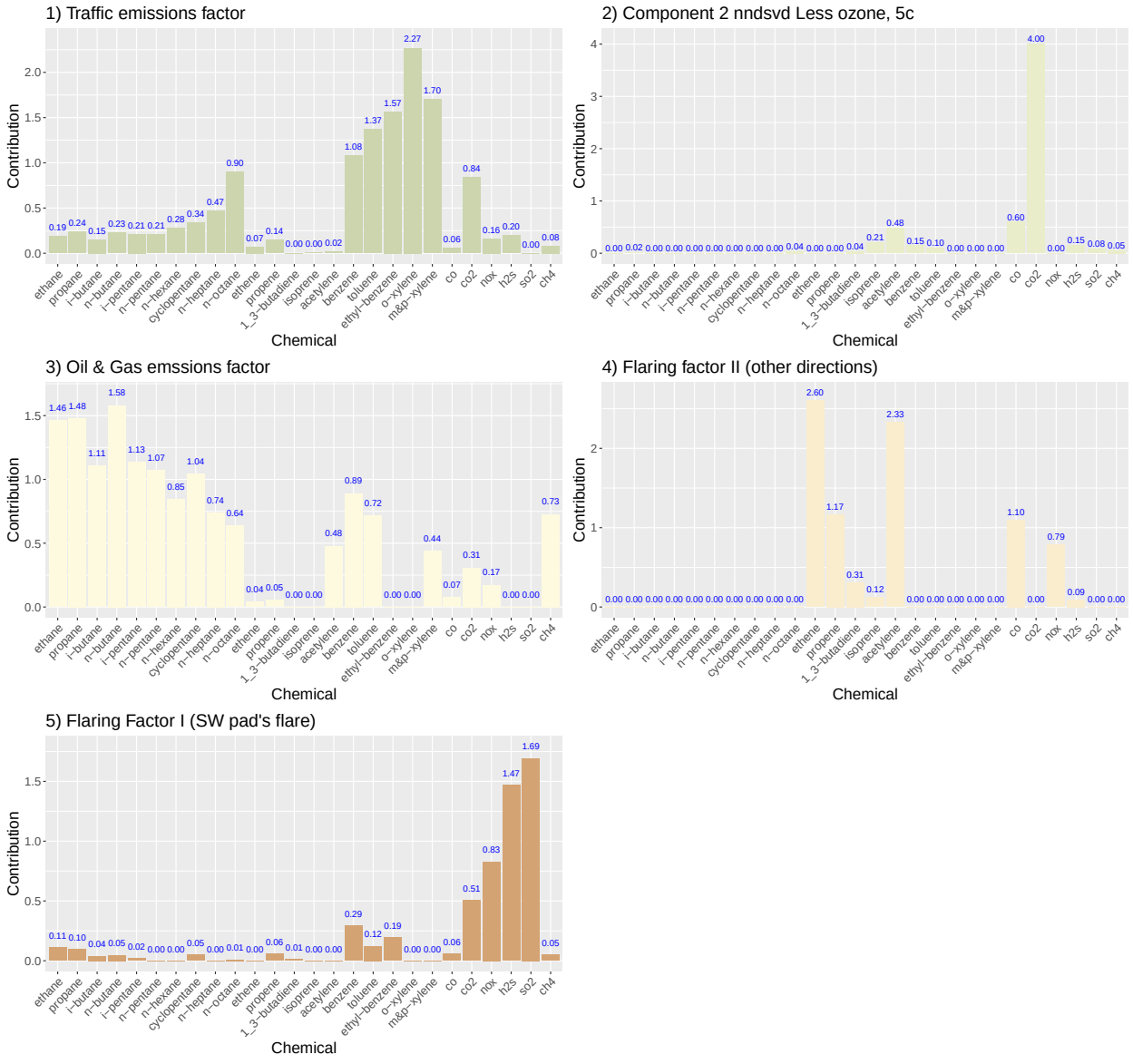
```
## Warning in sqrt(S[i] * termp) * uup: Recycling array of length 1 in array-vector arithmetic is depre
##   Use c() or as.vector() instead.

## Warning in sqrt(S[i] * termp) * vvp: Recycling array of length 1 in array-vector arithmetic is depre
##   Use c() or as.vector() instead.
```

```r
basis_matrix_5c_less_o3 <- basis(nmf_result_5c_less_o3)
coef_matrix_5c_less_o3 <- coef(nmf_result_5c_less_o3)

par(mfrow = c(1, 2))
image(basis_matrix_5c_less_o3, main = "Basis Matrix (W)")
image(coef_matrix_5c_less_o3, main = "Coefficient Matrix (H)")
```




```r
# Convert H to a data frame for ggplot
H_df_5c_less_o3 <- as.data.frame(coef_matrix_5c_less_o3)
# Add a column for chemicals
H_df_5c_less_o3$Component <- rownames(H_df_5c_less_o3)

# Reshape data to long format
H_long_5c_less_o3 <- pivot_longer(H_df_5c_less_o3, cols = -Component, names_to = "Chemical", values_to =

# Plot
nmfplt_1_svd_5c_less_o3 <- get_component_plot(H_long_5c_less_o3,
                                              '1', '1) Traffic emissions factor')
nmfplt_2_svd_5c_less_o3 <- get_component_plot(H_long_5c_less_o3,
```

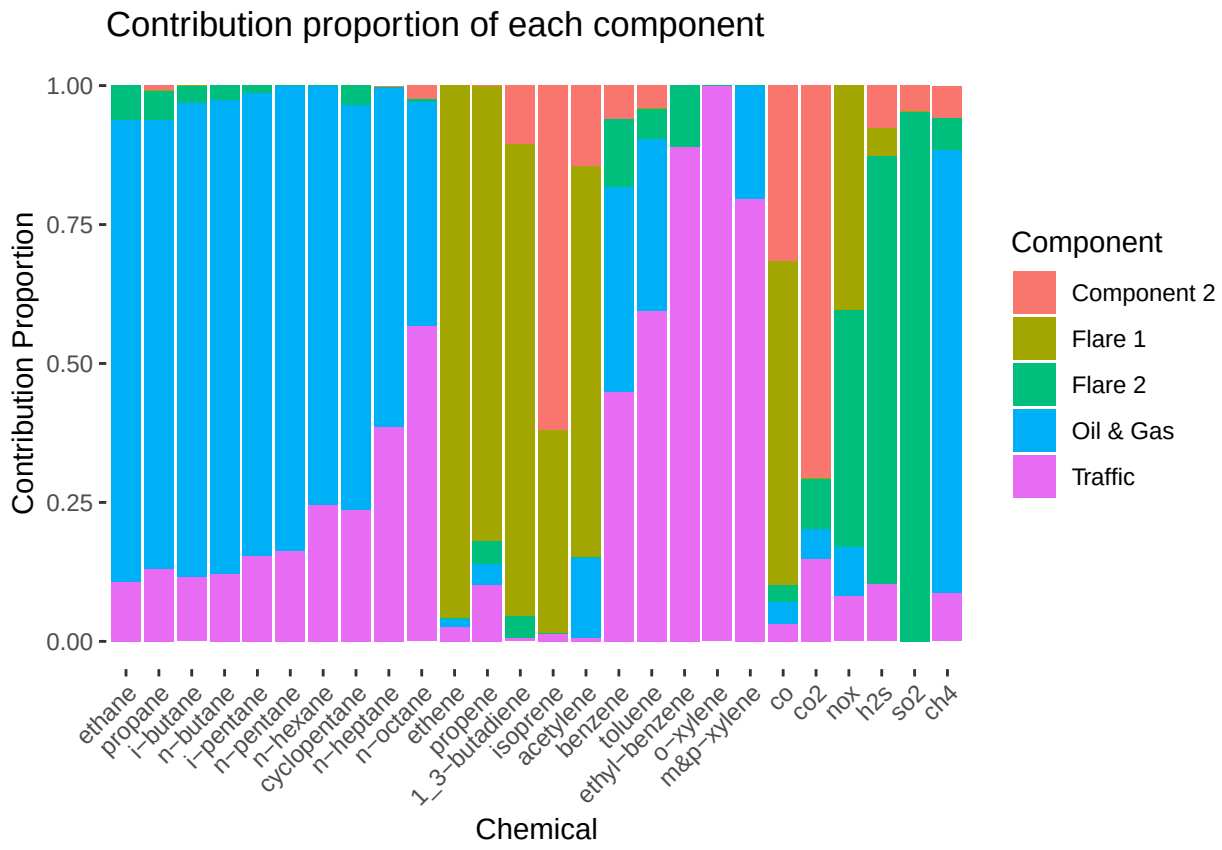
```
                                        '2', '2) Component 2 nndsvd Less ozone, 5c')
nmfplt_3_svd_5c_less_o3 <- get_component_plot(H_long_5c_less_o3,
                                        '3', '3) Oil & Gas emssions factor')
nmfplt_4_svd_5c_less_o3 <- get_component_plot(H_long_5c_less_o3,
                                        '4', '4) Flaring factor II (other directions)')
nmfplt_5_svd_5c_less_o3 <- get_component_plot(H_long_5c_less_o3,
                                        '5', '5) Flaring Factor I (SW pad\'s flare)')
```




## Fingerprint plot

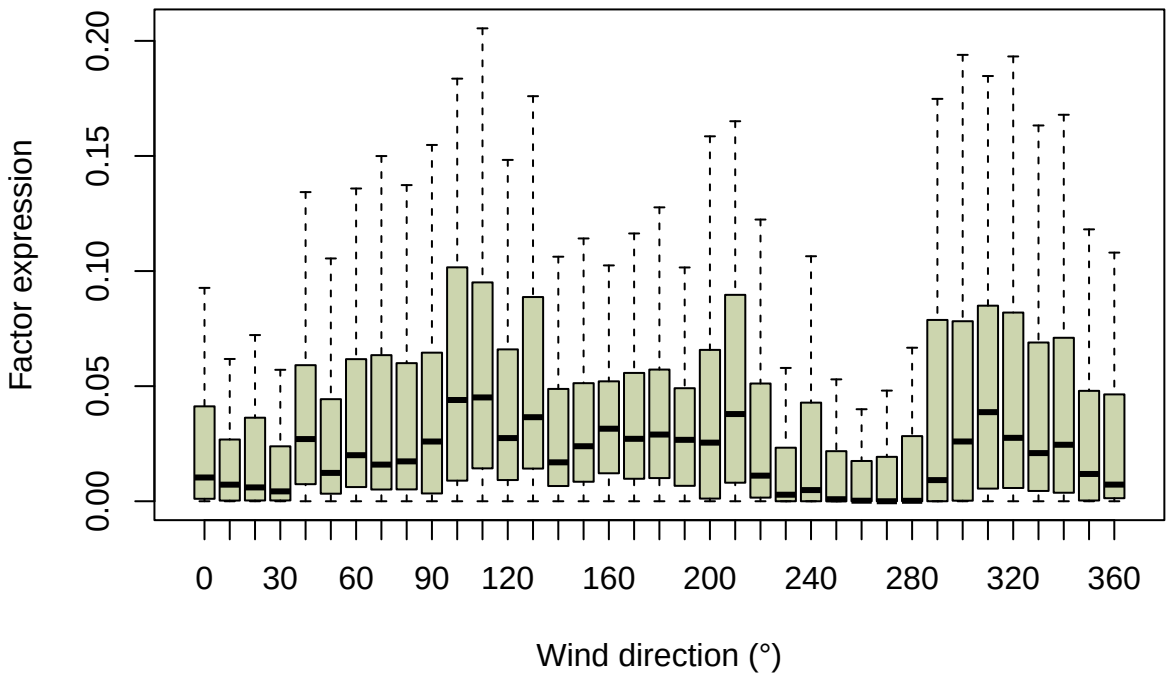
```
contrib_prop <- apply(H_df_5c_less_o3[,1:(length(H_df_5c_less_o3)-1)], MARGIN = 2, FUN = function(x) {x,
contrib_prop %>%
  as_tibble() %>%
  mutate(Component = c('Traffic', 'Component 2', 'Oil & Gas', 'Flare 1', 'Flare 2')) %>%
```

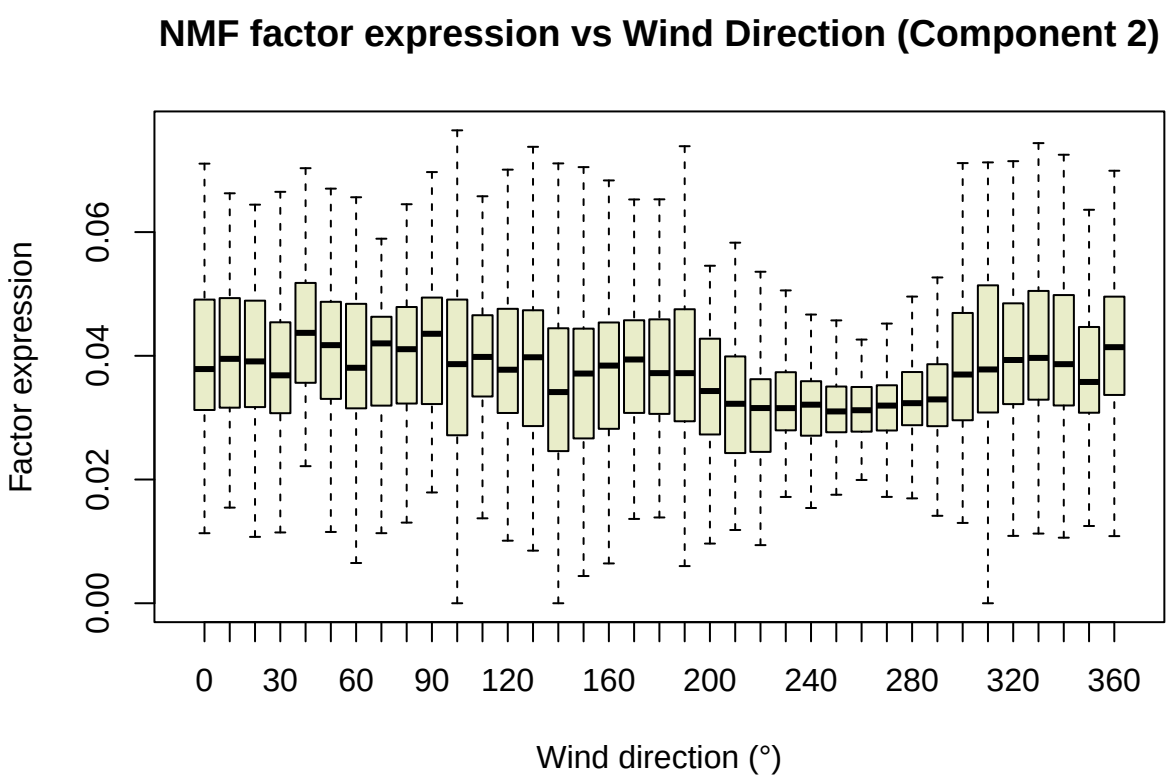
```
  pivot_longer(cols = -Component, names_to = "Chemical", values_to = "Contribution_prop") %>%
  mutate(Chemical = factor(Chemical, levels = desired_order)) %>%
  ggplot(aes(fill=Component, y=Contribution_prop, x=Chemical)) +
  geom_bar(position="fill", stat="identity") +
  theme(axis.text.x = element_text(angle = 45, hjust = 1)) +
  labs(x = "Chemical", y = "Contribution Proportion",
       title = 'Contribution proportion of each component') +
  theme(panel.grid.major = element_blank(),
        panel.grid.minor = element_blank(),
        panel.background = element_blank())
```

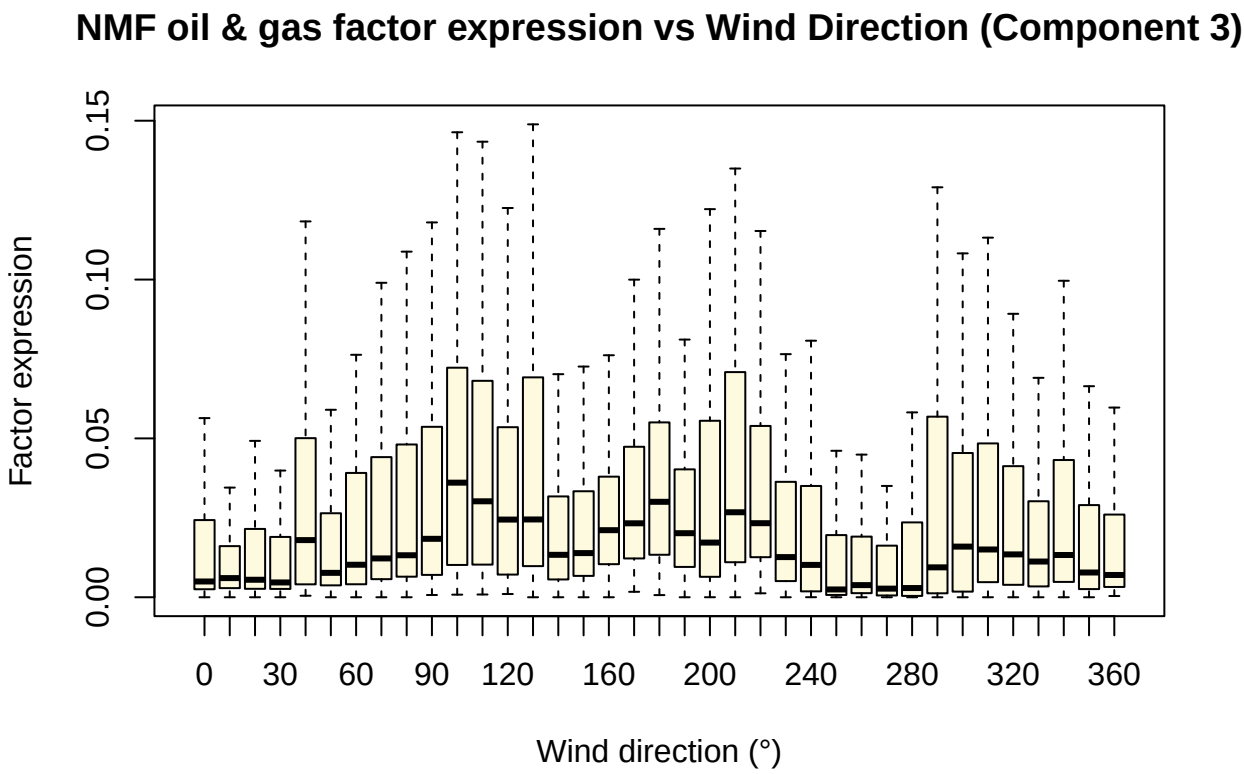


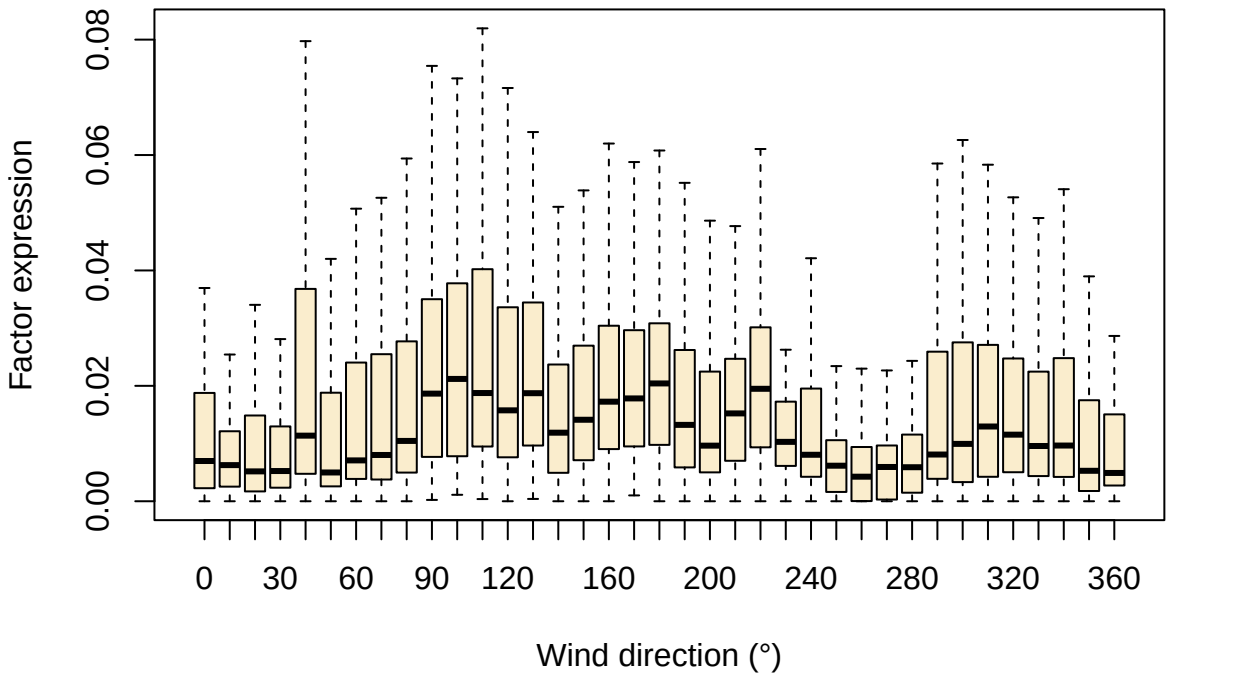

**Wind plots**

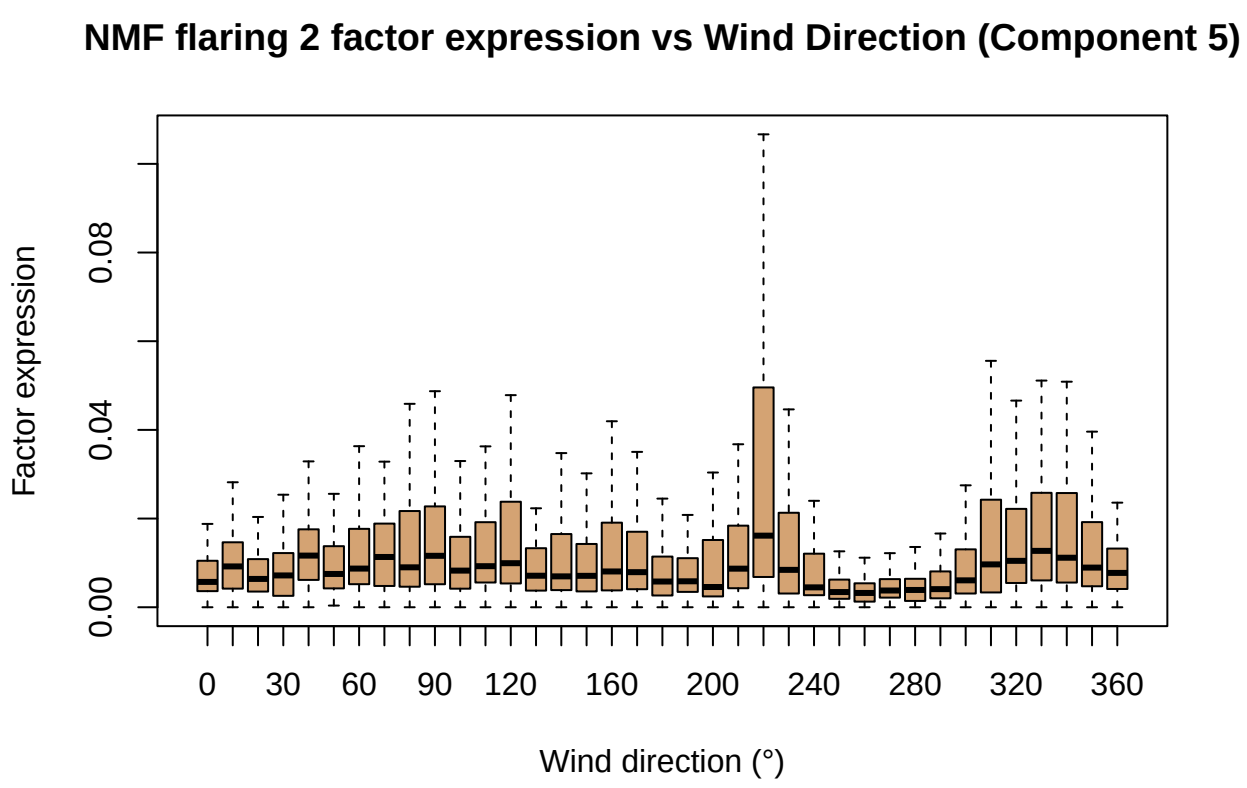
```
hourly_wind_nona <- hourly_nona %>%
  select(wdr_deg, wsp_ms)

data_to_plot <- tibble(
  component1 = basis(nmf_result_5c_less_o3)[,1],
  component2 = basis(nmf_result_5c_less_o3)[,2],
  component3 = basis(nmf_result_5c_less_o3)[,3],
  component4 = basis(nmf_result_5c_less_o3)[,4],
  component5 = basis(nmf_result_5c_less_o3)[,5],
  wd = round(hourly_wind_nona$wdr_deg, -1)
)
```


NMF traffic factor expression vs Wind Direction (Component 1)
Factor expression
0.00
0.05
0.10
0.15
0.20
0
30
60
90
120
160
200
240
280
320
360
Wind direction (°)


NMF factor expression vs Wind Direction (Component 2)
Factor expression
0.00
0.02
0.04
0.06
0
30
60
90
120
160
200
240
280
320
360
Wind direction (°)


NMF oil & gas factor expression vs Wind Direction (Component 3)
Factor expression
0.00
0.05
0.10
0.15
0
30
60
90
120
160
200
240
280
320
360
Wind direction (°)


NMF flaring 1 factor expression vs Wind Direction (Component 4)
Factor expression
0.00
0.02
0.04
0.06
0.08
0
30
60
90
120
160
200
240
280
320
360
Wind direction (°)




## Factor analysis

- merge in factors 1-5 to dataset (hourly)

```
# First look at how well this approximates
fitted_5c_less_o3 <- fitted(nmf_result_5c_less_o3)
sum(abs(normalized_matrix_less_o3-fitted_5c_less_o3))
```

```
## [1] 1060.414
```

```
# NMF factorizes V = WH
# Store Basis matrix (W) and Coef Matrix (H)
saveRDS(basis_matrix_5c_less_o3, 'result_rfiles/nmf_norm_5c_less_o3_basis.rds')
saveRDS(coef_matrix_5c_less_o3, 'result_rfiles/nmf_norm_5c_less_o3_coef.rds')

# Merge basis matrix into hourly observations
basis_matrix_5c_less_o3 <- as_tibble(basis_matrix_5c_less_o3) %>%
  setNames(c('Factor1', 'Factor2', 'Factor3', 'Factor4', 'Factor5'))
```

```
## Warning: The ‘x‘ argument of ‘as_tibble.matrix()‘ must have unique column names if
## ‘.name_repair‘ is omitted as of tibble 2.0.0.
## i Using compatibility ‘.name_repair‘.
## This warning is displayed once every 8 hours.
## Call ‘lifecycle::last_lifecycle_warnings()‘ to see where this warning was
## generated.
```

```r
normalized_hourly_data_5c_less_o3 <- hourly_nona[,c('day', 'time_utc')] %>%
  cbind(normalized_matrix_less_o3) %>%
  cbind(basis_matrix_5c_less_o3) %>%
  right_join(hourly_data %>% select(-'day'), join_by(time_utc), suffix = c('_norm', ''))

# saveRDS(normalized_hourly_data_5c_less_o3, 'result_rfiles/normalized_hourly_data_5c_less_o3.rds')
```

- make daily dataset for VNF analysis

```r
# Also compute a daily dataset
normalized_daily_data_5c_less_o3 <- normalized_hourly_data_5c_less_o3 %>%
  group_by(day) %>%
  summarise(across(where(is.numeric) & !any_of('wdr_deg'), ~ mean(.x, na.rm = T)),
            wdr_deg = as.numeric(mean(circular(wdr_deg, units = "degrees"), na.rm = T))) %>%
  mutate(wdr_deg = if_else(wdr_deg < 0, wdr_deg+360, wdr_deg)) %>%
  mutate(wind_45_135 = wdr_deg >= 45 & wdr_deg < 135,
         wind_135_180 = wdr_deg >= 135 & wdr_deg < 180,
         wind_180_270 = wdr_deg >= 180 & wdr_deg < 270,
         wind_270_45 = wdr_deg >= 270 & wdr_deg < 45)

# saveRDS(normalized_daily_data_5c_less_o3, 'result_rfiles/normalized_daily_data_5c_less_o3.rds')

normalized_daily_data_5c_less_o3 <- readRDS('result_rfiles/normalized_daily_data_5c_less_o3.rds')
```

- 1) number of flares in 100km of trailer associated with NMF
- 2) weighted cout based on distance to trailer

```r
# Check if relationship between # flares and flare factor (4 & 5)
# Linear model
flare_factor <- lm(n_flare_100 ~ Factor1 + Factor2 + Factor3 + Factor4 + Factor5, data = normalized_dai
summary(flare_factor)
```

```
##
## Call:
## lm(formula = n_flare_100 ~ Factor1 + Factor2 + Factor3 + Factor4 +
##     Factor5, data = normalized_daily_data_5c_less_o3)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -5.7635 -3.0378 -0.4893  2.3031 16.8406
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept)    3.351      1.014   3.305  0.00108 **
## Factor1      -10.434     14.475  -0.721  0.47163
## Factor2        7.936     26.825   0.296  0.76756
## Factor3       36.265     20.638   1.757  0.08001 .
## Factor4      -28.511     33.444  -0.852  0.39469
## Factor5       37.042     28.700   1.291  0.19791
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
```

```
## Residual standard error: 3.785 on 273 degrees of freedom
##   (1 observation deleted due to missingness)
## Multiple R-squared:  0.02441,    Adjusted R-squared:  0.006544
## F-statistic: 1.366 on 5 and 273 DF,  p-value: 0.2372
```

```
flare_factor45 <- lm(n_flare_100 ~ Factor4 + Factor5, data = normalized_daily_data_5c_less_o3)
summary(flare_factor45)
```

```
##
## Call:
## lm(formula = n_flare_100 ~ Factor4 + Factor5, data = normalized_daily_data_5c_less_o3)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -5.4658 -3.0946 -0.3795  2.2016 17.1266
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept)    3.592      0.456   7.878 7.71e-14 ***
## Factor4        6.625     20.357   0.325    0.745
## Factor5       42.500     27.706   1.534    0.126
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 3.787 on 276 degrees of freedom
##   (1 observation deleted due to missingness)
## Multiple R-squared:  0.01269,    Adjusted R-squared:  0.005536
## F-statistic: 1.774 on 2 and 276 DF,  p-value: 0.1716
```

```
flare_factor_weighted <- lm(weighted.count ~ Factor1 + Factor2 + Factor3 + Factor4 + Factor5, data = no
summary(flare_factor_weighted)
```

```
##
## Call:
## lm(formula = weighted.count ~ Factor1 + Factor2 + Factor3 + Factor4 +
##     Factor5, data = normalized_daily_data_5c_less_o3)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -10.369  -3.477  -0.572   2.114 117.655
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept)    9.165      2.232   4.107  5.3e-05 ***
## Factor1      -29.660     31.861  -0.931  0.35272
## Factor2     -121.718     59.043  -2.062  0.04020 *
## Factor3       20.457     45.425   0.450  0.65283
## Factor4      -43.619     73.613  -0.593  0.55398
## Factor5      188.812     63.171   2.989  0.00305 **
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 8.332 on 273 degrees of freedom
```

```
##   (1 observation deleted due to missingness)
## Multiple R-squared:  0.05585,    Adjusted R-squared:  0.03856
## F-statistic:  3.23 on 5 and 273 DF,  p-value: 0.007515
```

```
flare_factor_weighted45 <- lm(weighted.count ~ Factor4 + Factor5, data = normalized_daily_data_5c_less_
summary(flare_factor_weighted45)
```

```
##
## Call:
## lm(formula = weighted.count ~ Factor4 + Factor5, data = normalized_daily_data_5c_less_o3)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -10.209  -3.167  -0.377   1.832 120.250
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept)    5.030      1.007   4.996 1.04e-06 ***
## Factor4     -103.752     44.944  -2.308  0.02171 *
## Factor5      193.540     61.168   3.164  0.00173 **
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 8.361 on 276 degrees of freedom
##   (1 observation deleted due to missingness)
## Multiple R-squared:  0.03869,    Adjusted R-squared:  0.03173
## F-statistic: 5.554 on 2 and 276 DF,  p-value: 0.004316
```

```
# Wind direction from 270 to 45 is left as reference group.
flare_factor_weighted_2 <- lm(weighted.count ~ Factor1 + Factor2 + Factor3 + Factor4 + Factor5 + wsp_ms
summary(flare_factor_weighted_2)
```

```
##
## Call:
## lm(formula = weighted.count ~ Factor1 + Factor2 + Factor3 + Factor4 +
##     Factor5 + wsp_ms + wind_45_135 + wind_135_180 + Factor5 *
##     wind_180_270, data = normalized_daily_data_5c_less_o3)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -10.133  -3.436  -0.553   1.964 117.117
##
## Coefficients: (4 not defined because of singularities)
##                           Estimate Std. Error t value Pr(>|t|)
## (Intercept)                11.1536     3.1970   3.489 0.000566 ***
## Factor1                   -35.0200    32.4671  -1.079 0.281708
## Factor2                  -128.8912    59.6436  -2.161 0.031566 *
## Factor3                    12.0996    46.4525   0.260 0.794696
## Factor4                   -41.4700    73.6877  -0.563 0.574048
## Factor5                   184.9778    63.3537   2.920 0.003796 **
## wsp_ms                     -0.3760     0.4327  -0.869 0.385677
## wind_45_135TRUE                NA         NA      NA       NA
## wind_135_180TRUE               NA         NA      NA       NA
```

```
## wind_180_270TRUE                NA         NA      NA       NA
## Factor5:wind_180_270TRUE        NA         NA      NA       NA
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 8.335 on 272 degrees of freedom
##   (1 observation deleted due to missingness)
## Multiple R-squared:  0.05847,    Adjusted R-squared:  0.0377
## F-statistic: 2.815 on 6 and 272 DF,  p-value: 0.01128
```

```
# Wind direction from 270 to 45 is left as reference group.
flare_factor_weighted_3 <- lm(weighted.count ~ Factor4 + Factor5 + wsp_ms + wind_45_135 + wind_135_180 +
summary(flare_factor_weighted_3)
```

```
##
## Call:
## lm(formula = weighted.count ~ Factor4 + Factor5 + wsp_ms + wind_45_135 +
##     wind_135_180 + Factor5 * wind_180_270, data = normalized_daily_data_5c_less_o3)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -10.057  -3.206  -0.371   1.814 120.154
##
## Coefficients: (4 not defined because of singularities)
##                            Estimate Std. Error t value Pr(>|t|)
## (Intercept)                  5.7114     2.0994   2.720  0.00693 **
## Factor4                   -111.7978    49.9893  -2.236  0.02613 *
## Factor5                    190.1245    61.9557   3.069  0.00236 **
## wsp_ms                      -0.1466     0.3961  -0.370  0.71162
## wind_45_135TRUE                 NA         NA      NA       NA
## wind_135_180TRUE                NA         NA      NA       NA
## wind_180_270TRUE                NA         NA      NA       NA
## Factor5:wind_180_270TRUE        NA         NA      NA       NA
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 8.374 on 275 degrees of freedom
##   (1 observation deleted due to missingness)
## Multiple R-squared:  0.03917,    Adjusted R-squared:  0.02869
## F-statistic: 3.737 on 3 and 275 DF,  p-value: 0.01168
```

```
# Check relationship between avg flare distance and flare factor (4 & 5)
# Linear model
flare_factor_dist <- lm(distToLovi ~ Factor4 + Factor5, data = normalized_daily_data_5c_less_o3)
summary(flare_factor_dist)
```

```
##
## Call:
## lm(formula = distToLovi ~ Factor4 + Factor5, data = normalized_daily_data_5c_less_o3)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -17.8872  -4.0924  -0.6397   3.1281  15.8871
```

```
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept)  20.3055     0.8902  22.809   <2e-16 ***
## Factor4      78.3034    40.2421   1.946    0.053 .
## Factor5     -61.7593    51.8998  -1.190    0.235
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 6.536 on 218 degrees of freedom
##   (59 observations deleted due to missingness)
## Multiple R-squared:  0.01769,    Adjusted R-squared:  0.008681
## F-statistic: 1.963 on 2 and 218 DF,  p-value: 0.1429
```