Appendix A

Code for Part A

Import Necessary Libraries

```
In [87]: suppressWarnings({
    library(dplyr)
    library(xts)
    library(ggplot2)
    library(tidyr)
    })
```

Setting Working Directory

```
In [88]: path <- 'C:\\Users\\Aalok\\OneDrive - lamar.edu\\000Water_Q_Modelling\\WD'
    setwd(path)</pre>
```

Importing file with water quality parameters

```
In [89]: a <- read.csv('Combined_PIB_WQ.csv')
    colnames(a) <- c('Date', 'Time', 'TempC', 'Depth', 'SpCond', 'WatTurb', 'TDS', 'DisOx', '
    print(head(a))</pre>
```

```
Date Time TempC Depth SpCond WatTurb TDS DisOx pH 1 2008-07-01 00:00:00 27.6AQI 0.700AQI 173AQI 53.81AQI 112AQI 3.9AQI 6.7AQI 2 2008-07-01 00:15:00 27.5AQI 0.600AQI 175AQI 54.51AQI 114AQI 3.7AQI 6.6AQI 3 2008-07-01 00:30:00 27.5AQI 0.700AQI 175AQI 54.21AQI 114AQI 3.7AQI 6.6AQI 4 2008-07-01 00:45:00 27.4AQI 0.700AQI 175AQI 54.60AQI 114AQI 3.7AQI 6.6AQI 5 2008-07-01 01:00:00 27.4AQI 0.700AQI 174AQI 55.10AQI 113AQI 3.6AQI 6.7AQI 6 2008-07-01 01:15:00 27.4AQI 0.600AQI 175AQI 54.81AQI 114AQI 3.5AQI 6.6AQI
```

Reformatting date and time in a new column

```
In [90]: a$datetime <- paste(a$Date, a$Time)
   a$datetime <- as.POSIXct(a$datetime, format = "%Y-%m-%d %H:%M:%S")
   a$datetime <- format(a$datetime, "%d/%m/%Y %H:%M")
   head(a)</pre>
```

A data.frame: 6×10

	Date	Time	TempC	Depth	SpCond	WatTurb	TDS	DisOx	рН	datetime
	<chr></chr>									
1	2008-07-01	00:00:00	27.6AQI	0.700AQI	173AQI	53.81AQI	112AQI	3.9AQI	6.7AQI	01/07/2008 00:00
2	2008-07-01	00:15:00	27.5AQI	0.600AQI	175AQI	54.51AQI	114AQI	3.7AQI	6.6AQI	01/07/2008 00:15
3	2008-07-01	00:30:00	27.5AQI	0.700AQI	175AQI	54.21AQI	114AQI	3.7AQI	6.6AQI	01/07/2008 00:30
4	2008-07-01	00:45:00	27.4AQI	0.700AQI	175AQI	54.60AQI	114AQI	3.7AQI	6.6AQI	01/07/2008 00:45
5	2008-07-01	01:00:00	27.4AQI	0.700AQI	174AQI	55.10AQI	113AQI	3.6AQI	6.7AQI	01/07/2008 01:00
6	2008-07-01	01:15:00	27.4AQI	0.600AQI	175AQI	54.81AQI	114AQI	3.5AQI	6.6AQI	01/07/2008 01:15

Remove words from the dataframe and extract values only

```
In [91]:
        my_df <- a %>%
          mutate_at(vars('TempC','Depth','SpCond','WatTurb','TDS','DisOx','pH'), ~ as.numer
         print(head(my df))
                        Time TempC Depth SpCond WatTurb TDS DisOx pH
                Date
                                                                           datetime
        1 2008-07-01 00:00:00 27.6
                                           173
                                                 53.81 112 3.9 6.7 01/07/2008 00:00
                                     0.7
        2 2008-07-01 00:15:00 27.5
                                     0.6
                                           175
                                                 54.51 114 3.7 6.6 01/07/2008 00:15
                                           175
                                                 54.21 114 3.7 6.6 01/07/2008 00:30
        3 2008-07-01 00:30:00 27.5
                                     0.7
        4 2008-07-01 00:45:00 27.4
                                           175
                                                 54.60 114 3.7 6.6 01/07/2008 00:45
                                     0.7
        5 2008-07-01 01:00:00 27.4
                                           174
                                                 55.10 113 3.6 6.7 01/07/2008 01:00
                                     0.7
        6 2008-07-01 01:15:00 27.4
                                     0.6
                                           175
                                                 54.81 114
                                                            3.5 6.6 01/07/2008 01:15
```

Import the file with flow data

```
b <- read.csv('FlowData_15Min Interval.csv')</pre>
In [92]:
          print(head(b))
                                    datetime tz_cd flow_cfs
           agency_cd site_no
                USGS 8041749 1/10/2003 0:00
                                                CDT
                                                        -370
          2
                 USGS 8041749 1/10/2003 0:15
                                                CDT
                                                        -371
          3
                USGS 8041749 1/10/2003 0:30
                                                CDT
                                                        -290
                 USGS 8041749 1/10/2003 0:45
                                                CDT
                                                        -291
          5
                 USGS 8041749 1/10/2003 1:00
                                                CDT
                                                        -347
                 USGS 8041749 1/10/2003 1:15
                                                CDT
                                                        -376
```

Reformat DateTime

```
In [93]: b$datetime <- as.POSIXct(b$datetime, format = "%d/%m/%Y %H:%M")
b$datetime <- format(b$datetime, "%d/%m/%Y %H:%M")
print(head(b))</pre>
```

```
agency_cd site_no datetime tz_cd flow_cfs

1 USGS 8041749 01/10/2003 00:00 CDT -370

2 USGS 8041749 01/10/2003 00:15 CDT -371

3 USGS 8041749 01/10/2003 00:30 CDT -290

4 USGS 8041749 01/10/2003 00:45 CDT -291

5 USGS 8041749 01/10/2003 01:00 CDT -347

6 USGS 8041749 01/10/2003 01:15 CDT -376
```

Merging dataframes based on common column

```
In [94]: merged_df <- merge(b, my_df, by = "datetime", all = TRUE)
merged_df[5001:5005,]</pre>
```

		A data.frame: 5 × 14									
	datetime	agency_cd	site_no	tz_cd	flow_cfs	Date	Time	TempC	Depth	SpC	
	<chr></chr>	<chr></chr>	<int></int>	<chr></chr>	<dbl></dbl>	<chr></chr>	<chr></chr>	<dbl></dbl>	<dbl></dbl>	<c< th=""></c<>	
5001	01/03/2016 02:00	USGS	8041749	CST	-90.80	2016-03-01	02:00:00	17.1	0.887		
5002	01/03/2016 02:15	USGS	8041749	CST	-44.20	2016-03-01	02:15:00	17.1	0.883		
5003	01/03/2016 02:30	USGS	8041749	CST	-21.00	2016-03-01	02:30:00	17.0	0.877		
5004	01/03/2016 02:45	USGS	8041749	CST	-90.60	2016-03-01	02:45:00	17.0	0.872		
5005	01/03/2016 03:00	USGS	8041749	CST	2.26	2016-03-01	03:00:00	16.9	0.866		

Extracting parameters to find correlation into a separate dataframe

```
In [95]: df <- merged_df[, c("TempC","Depth","SpCond","WatTurb","TDS","DisOx","pH","flow_cfs</pre>
```

Removing Outliers

```
In [96]: df[df == 1000000] <- NA
    df$TempC[df$TempC > 10000] <- NA
    df$Depth[df$Depth > 30] <- NA
    df$SpCond[df$SpCond > 550] <- NA
    df$WatTurb[df$WatTurb > 500] <- NA
    df$TDS[df$TDS > 2500] <- NA
    df$DisOx[df$DisOx > 20] <- NA
    df$PH[df$pH > 14] <- NA</pre>
```

Calculate Correlation

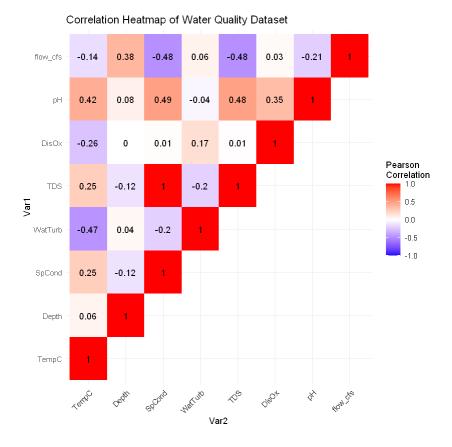
```
In [97]: cor_matrix <- cor(df, use = "pairwise.complete.obs")
    cor_matrix</pre>
```

A matrix: 8×8 of type dbl

	TempC	Depth	SpCond	WatTurb	TDS	DisOx	ķ
TempC	1.0000000	0.056179896	0.25485952	-0.46548762	0.254805523	-0.256702102	0.420396
Depth	0.0561799	1.000000000	-0.12469103	0.03643466	-0.124830216	-0.000760466	0.076696
SpCond	0.2548595	-0.124691028	1.00000000	-0.19981323	0.997919078	0.010456146	0.488304
WatTurb	-0.4654876	0.036434656	-0.19981323	1.00000000	-0.197628711	0.167101061	-0.038016
TDS	0.2548055	-0.124830216	0.99791908	-0.19762871	1.000000000	0.008783385	0.483775
DisOx	-0.2567021	-0.000760466	0.01045615	0.16710106	0.008783385	1.000000000	0.349921
рН	0.4203964	0.076696911	0.48830455	-0.03801656	0.483775202	0.349921933	1.000000
flow_cfs	-0.1446149	0.375503874	-0.48099239	0.06368365	-0.477728057	0.028991180	-0.209966

Plot Heatmap of correlation matrix

```
In [98]:
         # Create a lower triangular matrix with NA in the upper triangle
          lower_tri <- cor_matrix</pre>
          lower_tri[upper.tri(cor_matrix)] <- NA</pre>
          # Melt the lower triangular matrix and remove NA values
          library(reshape2)
          melted_cor <- melt(lower_tri, na.rm = TRUE)</pre>
          # Create a correlation heatmap using ggplot2
          ggplot(data = melted_cor, aes(x=Var2, y=Var1, fill=value, label = round(value, 2)))
           geom_tile() +
            geom_text(color = "black") +
            scale_fill_gradient2(low = "blue", mid = "white", high = "red",
                                 midpoint = 0, limit = c(-1,1), space = "Lab",
                                 name="Pearson\nCorrelation") +
            theme_minimal() +
            theme(axis.text.x = element_text(angle = 45, hjust = 1)) +
            ggtitle("Correlation Heatmap of Water Quality Dataset")
```



Preparing the dataframe with datetime to perform data aggregation

```
In [99]: df <- merged_df[, c("datetime","TempC","Depth","SpCond","WatTurb","TDS","DisOx","pH

#OutLier Removal

df[df == 1000000] <- NA

df$TempC[df$TempC > 10000] <- NA

df$Depth[df$Depth > 30] <- NA

df$SpCond[df$SpCond > 550] <- NA

df$WatTurb[df$WatTurb > 500] <- NA

df$TDS[df$TDS > 2500] <- NA

df$DisOx[df$DisOx > 20] <- NA

df$pH[df$pH > 14] <- NA</pre>
```

Remove rows without flow data and reformat datetime

```
In [100... df <- df[complete.cases(df$datetime), ]
    df$datetime <- as.POSIXct(df$datetime, format = "%d/%m/%Y %H:%M")</pre>
```

Convert to xts object with 15-minute intervals

```
In [101... xts_data <- xts(df[,2:9], order.by = df$datetime) #Line 2 to 9 includes all the par
```

Create hourly data aggregation and a respective dataframe

```
In [102... hourly_data <- aggregate(xts_data, as.POSIXct(cut(index(xts_data), breaks="hour")),
    hourly_df <- as.data.frame(hourly_data)</pre>
```

Create daily data aggregation and a respective dataframe

Create daily minimum data aggregation and a respective dataframe

```
In [104... daily_min <- aggregate(xts_data, as.Date(index(xts_data)), min)
    dailymin_df <- as.data.frame(daily_min)</pre>
```

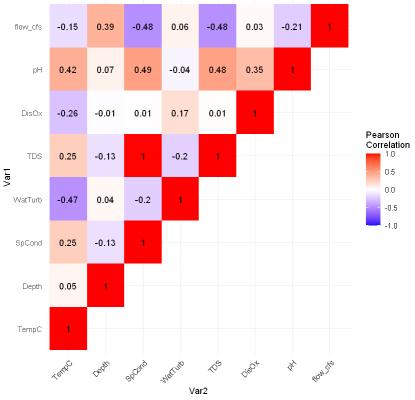
Create daily maximum data aggregation and a respective dataframe

Correlation for each aggregation scenario

Hourly Data

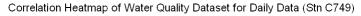
```
In [107...
          #Calculate correlation
           cor2 <- cor(hourly_df, use = "pairwise.complete.obs")</pre>
           # Create a lower triangular matrix with NA in the upper triangle
           lower_tri <- cor2</pre>
           lower_tri[upper.tri(cor2)] <- NA</pre>
           # Melt the lower triangular matrix and remove NA values
           melted_cor <- melt(lower_tri, na.rm = TRUE)</pre>
           # Create a correlation heatmap using ggplot2
           ggplot(data = melted_cor, aes(x=Var2, y=Var1, fill=value, label = round(value, 2)))
             geom_tile() +
             geom_text(color = "black") +
             scale_fill_gradient2(low = "blue", mid = "white", high = "red",
                                   midpoint = 0, limit = c(-1,1), space = "Lab",
                                   name="Pearson\nCorrelation") +
             theme_minimal() +
             theme(axis.text.x = element_text(angle = 45, hjust = 1)) +
             ggtitle("Correlation Heatmap of Water Quality Dataset for Hourly Data (Stn C749)"
```

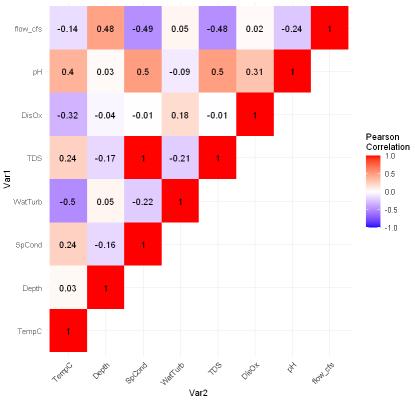




Daily Data

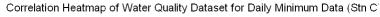
```
In [108...
          # Create a lower triangular matrix with NA in the upper triangle
          lower_tri <- cor3</pre>
          lower_tri[upper.tri(cor3)] <- NA</pre>
          # Melt the lower triangular matrix and remove NA values
          melted_cor <- melt(lower_tri, na.rm = TRUE)</pre>
          # Create a correlation heatmap using ggplot2
          ggplot(data = melted_cor, aes(x=Var2, y=Var1, fill=value, label = round(value, 2)))
            geom_tile() +
            geom_text(color = "black") +
             scale_fill_gradient2(low = "blue", mid = "white", high = "red",
                                  midpoint = 0, limit = c(-1,1), space = "Lab",
                                  name="Pearson\nCorrelation") +
            theme_minimal() +
             theme(axis.text.x = element_text(angle = 45, hjust = 1)) +
             ggtitle("Correlation Heatmap of Water Quality Dataset for Daily Data (Stn C749)")
```

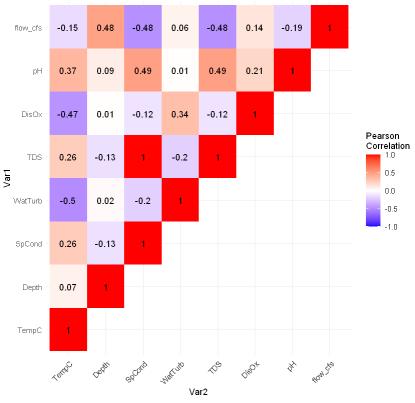




Daily Minimum Data

```
In [109...
          # Create a lower triangular matrix with NA in the upper triangle
          lower_tri <- cor4</pre>
          lower_tri[upper.tri(cor4)] <- NA</pre>
          # Melt the lower triangular matrix and remove NA values
          melted_cor <- melt(lower_tri, na.rm = TRUE)</pre>
          # Create a correlation heatmap using ggplot2
          ggplot(data = melted_cor, aes(x=Var2, y=Var1, fill=value, label = round(value, 2)))
            geom_tile() +
            geom_text(color = "black") +
             scale_fill_gradient2(low = "blue", mid = "white", high = "red",
                                  midpoint = 0, limit = c(-1,1), space = "Lab",
                                  name="Pearson\nCorrelation") +
            theme_minimal() +
             theme(axis.text.x = element_text(angle = 45, hjust = 1)) +
             ggtitle("Correlation Heatmap of Water Quality Dataset for Daily Minimum Data (Str
```





Daily Maximum Data

```
In [110...
          # Create a lower triangular matrix with NA in the upper triangle
          lower_tri <- cor5</pre>
          lower_tri[upper.tri(cor5)] <- NA</pre>
          # Melt the lower triangular matrix and remove NA values
          melted_cor <- melt(lower_tri, na.rm = TRUE)</pre>
          # Create a correlation heatmap using ggplot2
          ggplot(data = melted_cor, aes(x=Var2, y=Var1, fill=value, label = round(value, 2)))
            geom_tile() +
            geom_text(color = "black") +
             scale_fill_gradient2(low = "blue", mid = "white", high = "red",
                                  midpoint = 0, limit = c(-1,1), space = "Lab",
                                  name="Pearson\nCorrelation") +
            theme_minimal() +
             theme(axis.text.x = element_text(angle = 45, hjust = 1)) +
             ggtitle("Correlation Heatmap of Water Quality Dataset for Daily Maximum Data (Str
```



