CWRU DSCI351-351M-451 Class w05a: EDA of PET Sample Degradation (CWRU, Pitt, UCF, UTRGV)

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Contents

```r
# Reading and sorting files

# Always try to use `relative paths` to your files.
# "." is the current directory
# and ".." is one directory up, from the current directory
# As opposed to explicity, OS dependent paths, such as H:\Git....

# Try reading in a file to check the formatting and location
# "read.csv" does this well

dat <- read.csv("./data/sdle-sf/sdle-sf01_2013_12_24_0000.dat", skip = 1)

# create a vector of all files in this directory with the desired pattern
# list.files will give you a directory listing of the file names,

files <- list.files(path = "./data/sdle-sf/", pattern = "2013_12_24")
```

```r
# Define dat_total

dat_total <- NULL
i <- files[1]
# We can now use a for loop through all of the file names we want to read
for (i in files) {

  # read each file and remove the first 2 rows
  dat <- read.csv(paste0("./data/sdle-sf/", i), skip = 1)
  dat <- dat[-c(1,2),]

  # rbind data to organize it
  dat_total <- rbind(dat_total, dat)


}


library(tidyverse)
```

5.1.3.1 Reading and sorting files

```
## -- Attaching packages --------------------------------------- tidyverse 1.3.2 --
## v ggplot2 3.3.6      v purrr   0.3.4
## v tibble  3.1.8      v dplyr   1.0.10
## v tidyr   1.2.1      v stringr 1.4.1
## v readr   2.1.2      v forcats 0.5.2
## -- Conflicts ------------------------------------------ tidyverse_conflicts() --
## x dplyr::filter() masks stats::filter()
## x dplyr::lag()    masks stats::lag()
```

```
library(purrr)

dat_total2 <- NULL
dat_total2 <- files %>%
  map(~read_csv(file.path('data/sdle-sf/',.),skip = 3)) %>%
  reduce(rbind)
```

New names:
Rows: 113 Columns: 15
-- Column specification
--- Delimiter: "," dbl
(13): ...2, Avg...3, Tot, Avg...5, Avg...6, Max, Avg...9, Avg...10, Avg... dttm
(2): ...1, TMx
i Use `spec()` to retrieve the full column specification for this data. i
Specify the column types or set `show_col_types = FALSE` to quiet this message.
New names:
Rows: 112 Columns: 15
-- Column specification
--- Delimiter: "," dbl
(13): ...2, Avg...3, Tot, Avg...5, Avg...6, Max, Avg...9, Avg...10, Avg... dttm
(2): ...1, TMx
i Use `spec()` to retrieve the full column specification for this data. i
Specify the column types or set `show_col_types = FALSE` to quiet this message.
New names:
Rows: 104 Columns: 15
-- Column specification
--- Delimiter: "," dbl
(13): ...2, Avg...3, Tot, Avg...5, Avg...6, Max, Avg...9, Avg...10, Avg... dttm
(2): ...1, TMx
i Use `spec()` to retrieve the full column specification for this data. i
Specify the column types or set `show_col_types = FALSE` to quiet this message.
New names:
Rows: 108 Columns: 15
-- Column specification
--- Delimiter: "," dbl
(13): ...2, Avg...3, Tot, Avg...5, Avg...6, Max, Avg...9, Avg...10, Avg... dttm
(2): ...1, TMx
i Use `spec()` to retrieve the full column specification for this data. i
Specify the column types or set `show_col_types = FALSE` to quiet this message.
New names:
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(13): ...2, Avg...3, Tot, Avg...5, Avg...6, Max, Avg...9, Avg...10, Avg... dttm
(2): ...1, TMx
i Use `spec()` to retrieve the full column specification for this data. i
Specify the column types or set `show_col_types = FALSE` to quiet this message.
New names:
Rows: 107 Columns: 15
-- Column specification
--- Delimiter: "," dbl
(13): ...2, Avg...3, Tot, Avg...5, Avg...6, Max, Avg...9, Avg...10, Avg... dttm
(2): ...1, TMx
i Use `spec()` to retrieve the full column specification for this data. i
```

```
## Specify the column types or set `show_col_types = FALSE` to quiet this message.
## New names:
## Rows: 110 Columns: 15
## -- Column specification
## --------------------------------------------------------- Delimiter: "," dbl
## (13): ...2, Avg...3, Tot, Avg...5, Avg...6, Max, Avg...9, Avg...10, Avg... dttm
## (2): ...1, TMx
## i Use `spec()` to retrieve the full column specification for this data. i
## Specify the column types or set `show_col_types = FALSE` to quiet this message.
## New names:
## Rows: 110 Columns: 15
## -- Column specification
## --------------------------------------------------------- Delimiter: "," dbl
## (13): ...2, Avg...3, Tot, Avg...5, Avg...6, Max, Avg...9, Avg...10, Avg... dttm
## (2): ...1, TMx
## i Use `spec()` to retrieve the full column specification for this data. i
## Specify the column types or set `show_col_types = FALSE` to quiet this message.
## New names:
## Rows: 108 Columns: 15
## -- Column specification
## --------------------------------------------------------- Delimiter: "," dbl
## (13): ...2, Avg...3, Tot, Avg...5, Avg...6, Max, Avg...9, Avg...10, Avg... dttm
## (2): ...1, TMx
## i Use `spec()` to retrieve the full column specification for this data. i
## Specify the column types or set `show_col_types = FALSE` to quiet this message.
## New names:
## Rows: 110 Columns: 15
## -- Column specification
## --------------------------------------------------------- Delimiter: "," dbl
## (13): ...2, Avg...3, Tot, Avg...5, Avg...6, Max, Avg...9, Avg...10, Avg... dttm
## (2): ...1, TMx
## i Use `spec()` to retrieve the full column specification for this data. i
## Specify the column types or set `show_col_types = FALSE` to quiet this message.
## New names:
## Rows: 113 Columns: 15
## -- Column specification
## --------------------------------------------------------- Delimiter: "," dbl
## (13): ...2, Avg...3, Tot, Avg...5, Avg...6, Max, Avg...9, Avg...10, Avg... dttm
## (2): ...1, TMx
## i Use `spec()` to retrieve the full column specification for this data. i
## Specify the column types or set `show_col_types = FALSE` to quiet this message.
## New names:
## Rows: 112 Columns: 15
## -- Column specification
## --------------------------------------------------------- Delimiter: "," dbl
## (13): ...2, Avg...3, Tot, Avg...5, Avg...6, Max, Avg...9, Avg...10, Avg... dttm
## (2): ...1, TMx
## i Use `spec()` to retrieve the full column specification for this data. i
## Specify the column types or set `show_col_types = FALSE` to quiet this message.
## * `` -> `...1`
## * `` -> `...2`
## * `Avg` -> `Avg...3`
## * `Avg` -> `Avg...5`
## * `Avg` -> `Avg...6`
```

```
## * `Avg` -> `Avg...9`
## * `Avg` -> `Avg...10`
## * `Avg` -> `Avg...11`
## * `Avg` -> `Avg...12`
## * `Avg` -> `Avg...13`
## * `Avg` -> `Avg...14`
## * `Avg` -> `Avg...15`
```

```
names(dat_total2)[c(1,2)] <- names(dat)[c(1,2)]
# "rbind" is row bind, and "cbind" is column bind
```

5.1.3.2 Degradation of Polyester Films

- This is a Materials Data Science Study
- A Journal Article by Abdulkerim Gok
- Is located in 3-readings/4-MatSci-And-SemProjReadings/ folder of your class repo
  - "Gok et al. - 2017 - Predictive models of poly(ethylene-terephthalate).pdf"
- And the data set is summarized in 2-class/data
  - "PetDegr-DataFrameColumnDefinitions.pdf"

5.1.3.3 Study Design and Protocol

5.1.3.3.1 Samples

- Three PET grades used in this study are

  - Unstabilized PET: Melinex 454 (3 mils film thickness)
  - UV stabilized PET: Tetoron HB3 (2 mils film thickness)
  - Hyrolytically stabilized PET: Mitsubishi 8HL1 (5 mils film thickness)

5.1.3.3.2 Exposures

- Four different accelerated weathering exposures were applied:

Exposure	Condition
Continuous UVA	Constant exposure of 1.55 W/m^2 at 340nm at 70ºC
ASTM G154-4	Cyclic exposure of 8 hours of UVA light at 1.55 W/m^2 at 340nm at 70ºC and 4 hours of condensing humidity at 50ºC in the dark
Damp Heat	Constant exposure 85ºC / 85% RH exposure per IEC 61215
Humidity Freeze	Cyclic exposure of 70ºC / 85% RH and -40ºC per IEC 61215

5.1.3.3.3 Evaluations

- Three evaluation techniques are:

  - $L^*a^*b^*$ color, Yellowness index (YI) and Haze (%) measurements
    * using Hunterlabs UltrascanPro
  - Optical absorbance measurements (Abs) using Cary 6000i with DRA
    * DRA is a Diffuse Reflectance Attachment, or "Integrating Sphere"
  - IR spectra measurements using Agilent 630 FTIR with Diamond ATR

5.1.3.4 Raw Data: Optical Absorbance

- An example of raw spectra that comes right out of the instrument

  - Note the saturation of Absorbance for wavelengths below 300 nm

Figure 1: Figure

Figure 2: Figure. Note that the absorbance saturates for wavlengths < approx. 400 nm

5.1.3.4.1 Raw Data: Transmission

- An example of raw spectra that comes right out of the instrument
  - Note the saturation of Absorbance for wavelengths below 300 nm

Figure 3: Figure

An example of raw spectra that comes right out of the instrument

- Note the saturation of Absorbance for wavelengths below 300 nm

5.1.3.5 Processing Data

- Optical Absorbance is first normalized to thickness (abs/cm)
  - Then zero correction is applied between 600 and 800 nm
- Average "Induced Absorbance to Dose" (IAD) is calculated from corrected **abs/cm**
  - Negative IAD is photobleaching
  - Positive IAD is photodarkening

$$\frac{Abs}{cm} per \frac{GJ}{m^2} = aIAD = \frac{Abs_i(\lambda) - Abs_0(\lambda))}{Dose_i - Dose_0}$$

5.1.3.5.1 Point-in-Time Data

- Single values are extracted from spectra
  - YI and $Haze$ are already obtained directly from instruments

Single abs/cm values are extracted from spectra at specific wavelengths

  - Fundamental absorption edge at ~300 nm

  - Features associated with UV stabilizer at 335 nm, 350 nm, and 370 nm

  - Optical density at 400 nm related to yellowing
  - Single $aveIAD$ values are also extracted at the same wavelengths

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Figure 4: Figure

5.1.3.5.2 Point in Time Data

- Single values are extracted from spectra

  - Zero absorbance correction applied for FTIR between 4000-3500 cm^{-1} to remove offset

    * Single IR peak heights are extracted at specific wavenumbers
      · 714 cm^{-1} and 1017 cm^{-1} for out of plane and in plane vibration of benzene
      · 872 cm^{-1} and 1341 cm^{-1} for CH$_2$ rocking and wagging of glycol
      · 1093 cm^{-1}, 1251 cm^{-1}, and 1716 cm^{-1} for ester C=O stretching
    * Due to shifts in peak position,
      · maximum data point is pulled as the single data point in some range for the corresponding peaks
      · i.e., for the 1716 cm^{-1} data point, the maximum between 1700 cm^{-1} and 1730 cm^{-1} is extracted.

5.1.3.6 Data Structure Build the data frame for analysis

- All data put together in one data frame

  - Samples entered as rows and variables as columns:
    * Sample and exposure information (type, time and step size, irradiation and dose content, etc.)
    * Cyclic exposure conditions (rate of change from one state to another) for further modelling purposes
    * Spectral information, point in time, extracted from spectra
    * Spectra from UV-Vis (abs/cm) and IR also included.

5.1.3.6.1 Data Structure

- Introducing data frame:

```
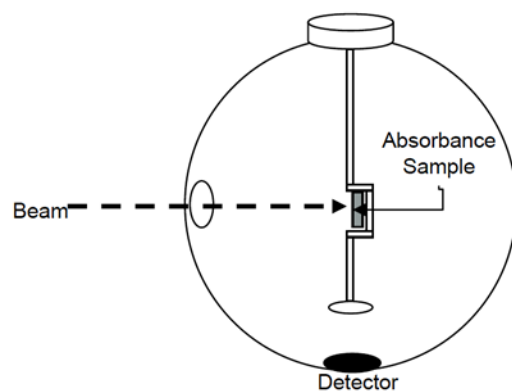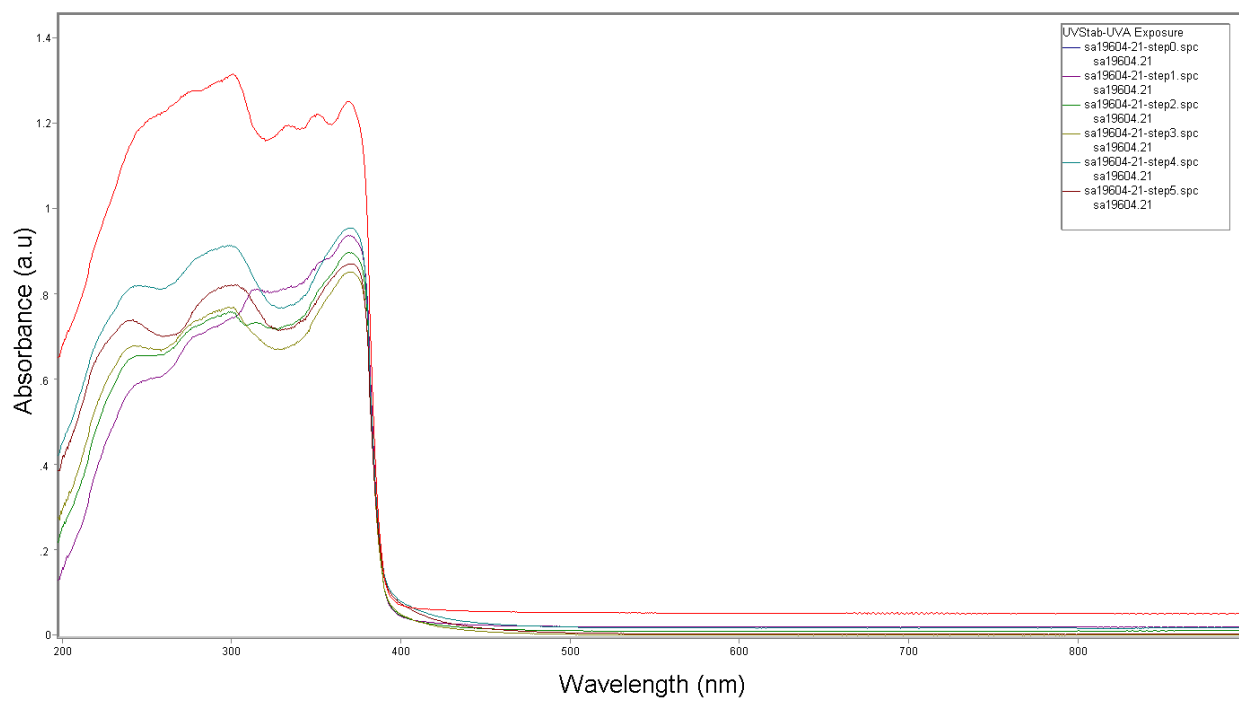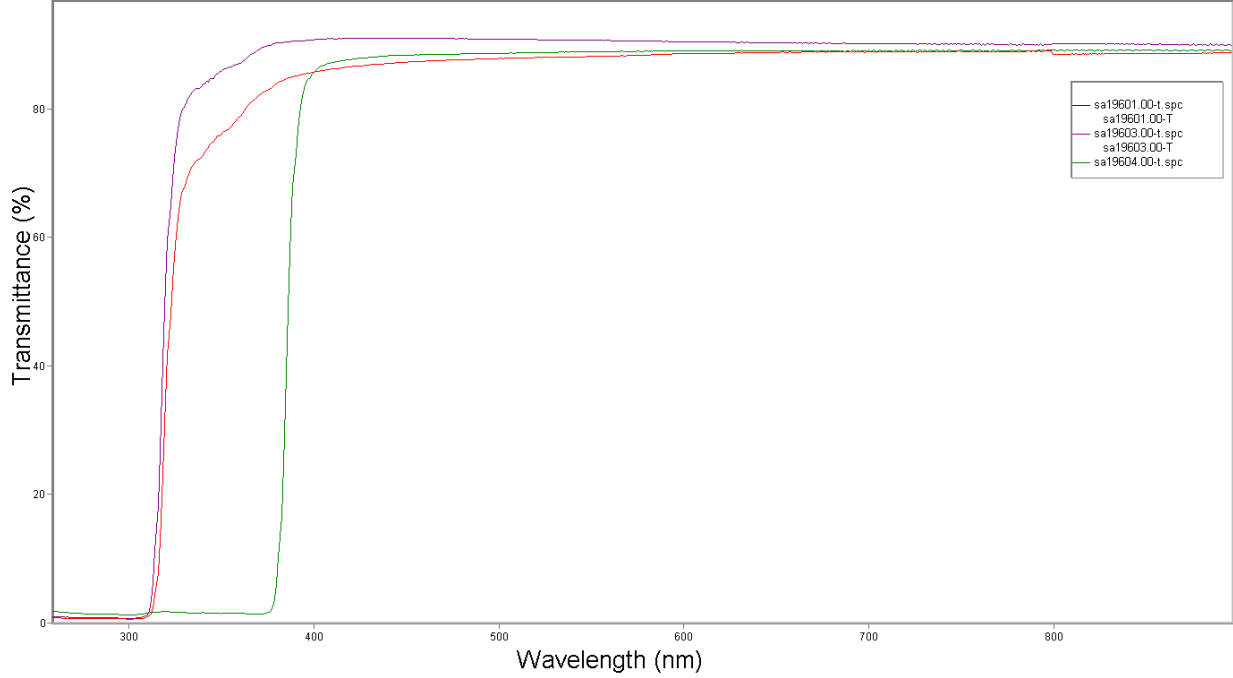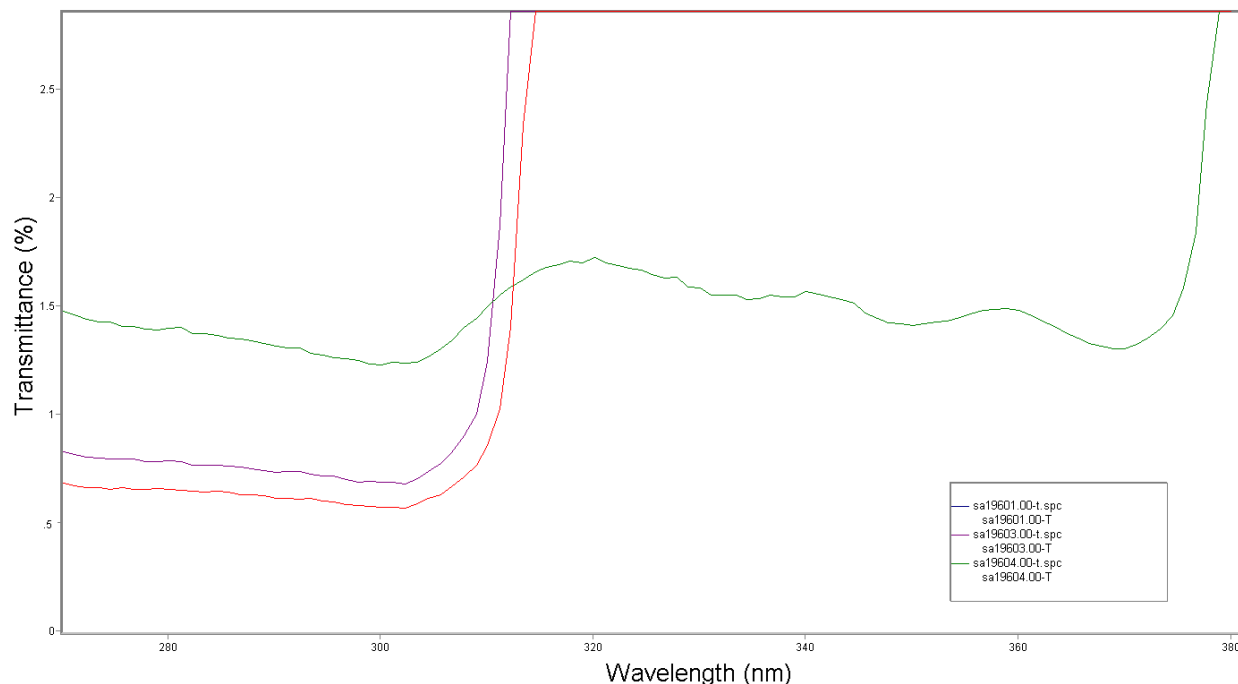library(tidyverse)
dat <- read.csv("../2-class/data/PetDegr-DataFrame-v05-singles.csv")
names(dat)
```

```
##  [1] "Rowkey"   "Sample"   "Material" "Thick"    "Exposure" "Time"
##  [7] "Step"     "Irrad"    "Pdose"    "L"        "a"        "b"
## [13] "YI"       "Haze"     "abs300"   "abs335"   "abs345"   "abs350"
## [19] "abs370"   "abs400"   "iad300"   "iad335"   "iad345"   "iad350"
## [25] "iad370"   "iad400"   "ftir1716" "ftir1409" "ftir1341" "ftir1251"
## [31] "ftir1093" "ftir1017" "ftir872"  "ftir714"
```

```
str(dat)
```

5.1.3.6.2 Data Structure

```
## 'data.frame':    405 obs. of  34 variables:
##  $ Rowkey  : chr  "sa19601.00-step0" "sa19601.01-step0" "sa19601.02-step0" "sa19601.03-step0" ...
##  $ Sample  : chr  "sa19601.00" "sa19601.01" "sa19601.02" "sa19601.03" ...
##  $ Material: chr  "HydStab" "HydStab" "HydStab" "HydStab" ...
##  $ Thick   : num  0.0125 0.0125 0.0125 0.0125 0.0125 0.0125 0.0125 0.0125 0.0125 0.0125 ...
##  $ Exposure: chr  "Baseline" "DampHeat" "DampHeat" "DampHeat" ...
##  $ Time    : int  0 0 0 0 0 0 0 0 0 0 ...
##  $ Step    : int  0 0 0 0 0 0 0 0 0 0 ...
##  $ Irrad   : num  NA 0 0 0 0 0 0 0 0 0 ...
##  $ Pdose   : num  NA 0 0 0 0 0 0 0 0 0 ...
##  $ L       : num  94.8 95.1 95.1 95.1 95.1 ...
##  $ a       : num  0 0 0 0 0 0.01 0.01 0.01 0.02 0 ...
##  $ b       : num  0.79 0.75 0.73 0.73 0.74 0.75 0.74 0.76 0.74 0.74 ...
##  $ YI      : num  1.5 1.42 1.39 1.38 1.4 1.44 1.42 1.44 1.42 1.4 ...
##  $ Haze    : num  3.8 0.8 1 1.4 0.9 0.9 1.2 1.3 2.4 1.8 ...
##  $ abs300  : num  NA 71.6 95.4 91.2 71.7 ...
##  $ abs335  : num  NA 4.62 5.44 5.5 4.6 ...
##  $ abs345  : num  NA 3.33 4.06 4.12 3.44 ...
##  $ abs350  : num  NA 3.1 3.76 3.74 3.09 ...
##  $ abs370  : num  NA 1.46 2.02 2.02 1.47 ...
##  $ abs400  : num  NA 0.302 0.648 0.685 0.312 ...
##  $ iad300  : num  NA NA NA NA NA NA NA NA NA NA ...
##  $ iad335  : num  NA NA NA NA NA NA NA NA NA NA ...
##  $ iad345  : num  NA NA NA NA NA NA NA NA NA NA ...
##  $ iad350  : num  NA NA NA NA NA NA NA NA NA NA ...
##  $ iad370  : num  NA NA NA NA NA NA NA NA NA NA ...
##  $ iad400  : num  NA NA NA NA NA NA NA NA NA NA ...
##  $ ftir1716: num  0.585 0.622 0.604 0.481 0.448 ...
##  $ ftir1409: num  0.186 0.189 0.188 0.164 0.156 ...
##  $ ftir1341: num  0.21 0.216 0.212 0.185 0.177 ...
##  $ ftir1251: num  0.621 0.663 0.643 0.522 0.491 ...
##  $ ftir1093: num  0.582 0.619 0.602 0.503 0.477 ...
##  $ ftir1017: num  0.391 0.408 0.399 0.353 0.342 ...
##  $ ftir872 : num  0.409 0.429 0.418 0.37 0.358 ...
##  $ ftir714 : num  0.871 0.933 0.903 0.793 0.77 ...
```

5.1.3.6.3 Data Structure

- Introducing data frame:

```
head(dat)[1:8]
```

```
##              Rowkey     Sample Material  Thick Exposure Time Step Irrad
## 1 sa19601.00-step0 sa19601.00  HydStab 0.0125 Baseline    0    0    NA
## 2 sa19601.01-step0 sa19601.01  HydStab 0.0125 DampHeat    0    0     0
## 3 sa19601.02-step0 sa19601.02  HydStab 0.0125 DampHeat    0    0     0
## 4 sa19601.03-step0 sa19601.03  HydStab 0.0125 DampHeat    0    0     0
## 5 sa19601.04-step0 sa19601.04  HydStab 0.0125 DampHeat    0    0     0
## 6 sa19601.05-step0 sa19601.05  HydStab 0.0125 DampHeat    0    0     0
```

```
tail(dat)[1:8]
```

```
##                Rowkey     Sample Material Thick   Exposure Time Step Irrad
## 400 sa19604.13-step6 sa19604.13   UVStab 0.005 FreezeThaw 1008    6  0.00
## 401 sa19604.14-step6 sa19604.14   UVStab 0.005 FreezeThaw 1008    6  0.00
## 402 sa19604.20-step6 sa19604.20   UVStab 0.005     HotQUV 1008    6  1.55
## 403 sa19604.21-step6 sa19604.21   UVStab 0.005     HotQUV 1008    6  1.55
## 404 sa19604.27-step6 sa19604.27   UVStab 0.005  CyclicQUV 1008    6  1.55
## 405 sa19604.28-step6 sa19604.28   UVStab 0.005  CyclicQUV 1008    6  1.55
```

```
glimpse(dat)
```

```
## Rows: 405
## Columns: 34
## $ Rowkey   <chr> "sa19601.00-step0", "sa19601.01-step0", "sa19601.02-step0", "~
## $ Sample   <chr> "sa19601.00", "sa19601.01", "sa19601.02", "sa19601.03", "sa19~
## $ Material <chr> "HydStab", "HydStab", "HydStab", "HydStab", "HydStab", "HydSt~
## $ Thick    <dbl> 0.0125, 0.0125, 0.0125, 0.0125, 0.0125, 0.0125, 0.0125, 0.012~
## $ Exposure <chr> "Baseline", "DampHeat", "DampHeat", "DampHeat", "DampHeat", "~
## $ Time     <int> 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0~
## $ Step     <int> 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0~
## $ Irrad    <dbl> NA, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.0~
## $ Pdose    <dbl> NA, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, ~
## $ L        <dbl> 94.82, 95.10, 95.10, 95.12, 95.09, 95.10, 95.08, 95.07, 95.02~
## $ a        <dbl> 0.00, 0.00, 0.00, 0.00, 0.00, 0.01, 0.01, 0.01, 0.02, 0.00, 0~
## $ b        <dbl> 0.79, 0.75, 0.73, 0.73, 0.74, 0.75, 0.74, 0.76, 0.74, 0.74, 0~
## $ YI       <dbl> 1.50, 1.42, 1.39, 1.38, 1.40, 1.44, 1.42, 1.44, 1.42, 1.40, 1~
## $ Haze     <dbl> 3.8, 0.8, 1.0, 1.4, 0.9, 0.9, 1.2, 1.3, 2.4, 1.8, 1.0, 0.9, 0~
## $ abs300   <dbl> NA, 71.64737, 95.42489, 91.24334, 71.74143, 70.53953, 71.7276~
## $ abs335   <dbl> NA, 4.617307, 5.440763, 5.501046, 4.595147, 4.631772, 4.70607~
## $ abs345   <dbl> NA, 3.333822, 4.061444, 4.118899, 3.442625, 3.396192, 3.48389~
## $ abs350   <dbl> NA, 3.102395, 3.758074, 3.738013, 3.088704, 3.122447, 3.21495~
## $ abs370   <dbl> NA, 1.455391, 2.022005, 2.023872, 1.472509, 1.504090, 1.54515~
## $ abs400   <dbl> NA, 0.3022738, 0.6477339, 0.6849267, 0.3117588, 0.3519749, 0.~
## $ iad300   <dbl> NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, N~
## $ iad335   <dbl> NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, N~
## $ iad345   <dbl> NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, N~
## $ iad350   <dbl> NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, N~
## $ iad370   <dbl> NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, N~
## $ iad400   <dbl> NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, N~
## $ ftir1716 <dbl> 0.5853787, 0.6223908, 0.6044577, 0.4805836, 0.4483261, 0.5620~
## $ ftir1409 <dbl> 0.1864237, 0.1886268, 0.1876017, 0.1638516, 0.1564671, 0.1810~
## $ ftir1341 <dbl> 0.2095117, 0.2156388, 0.2121917, 0.1853156, 0.1767081, 0.2040~
## $ ftir1251 <dbl> 0.6206618, 0.6625348, 0.6434837, 0.5218656, 0.4914321, 0.6078~
## $ ftir1093 <dbl> 0.5820087, 0.6187258, 0.6018527, 0.5032876, 0.4770921, 0.5716~
```

```
## $ ftir1017 <dbl> 0.3905907, 0.4077378, 0.3988337, 0.3529786, 0.3415001, 0.3844~
## $ ftir872  <dbl> 0.4085448, 0.4290438, 0.4180947, 0.3696016, 0.3576791, 0.4070~
## $ ftir714  <dbl> 0.8713277, 0.9332078, 0.9025477, 0.7928086, 0.7703331, 0.8938~
```

5.1.3.7   Data Subsetting

- Since we have three different materials

```r
library(dplyr)

unstab <- filter(dat, Material == 'Unstab')
# unstab <- dat[which(dat$Material=="Unstab"), ]

uvstab <- filter(dat, Material == 'UVStab')
# uvstab <- dat[which(dat$Material=="UVStab"), ]

hystab <- filter(dat, Material == 'HydStab')
# hystab <- dat[which(dat$Material=="HydStab"), ]
```

You can also use "subset" function to subset your data

```r
unstab.dh2 <- subset(dat, Material == "Unstab" & Exposure == "DampHeat")

uvstab.hq2 <- subset(dat, Material == "UVStab" & Exposure == "HotQUV")

hystab.ft2 <- subset(dat, Material == "HydStab" & Exposure == "FreezeThaw")
```

5.1.3.7.1   Data Subsetting

- Since we have four different exposures

```r
# Exposures for Unstabilized

unstab.dh <- filter(unstab, Exposure == "DampHeat")
unstab.ft <- filter(unstab, Exposure == "FreezeThaw")
unstab.hq <- filter(unstab, Exposure == "HotQUV")
unstab.cq <- filter(unstab, Exposure == "CyclicQUV")
# unstab.dh <- unstab[which(unstab$Exposure=="DampHeat"), ]
# unstab.ft <- unstab[which(unstab$Exposure=="FreezeThaw"), ]
# unstab.hq <- unstab[which(unstab$Exposure=="HotQUV"), ]
# unstab.cq <- unstab[which(unstab$Exposure=="CyclicQUV"), ]

# Exposures for UV stabilized

uvstab.dh <- filter(uvstab, Exposure == "DampHeat")
uvstab.ft <- filter(uvstab, Exposure == "FreezeThaw")
uvstab.hq <- filter(uvstab, Exposure == "HotQUV")
uvstab.cq <- filter(uvstab, Exposure == "CyclicQUV")
# uvstab.dh <- uvstab[which(uvstab$Exposure=="DampHeat"), ]
# uvstab.ft <- uvstab[which(uvstab$Exposure=="FreezeThaw"), ]
# uvstab.hq <- uvstab[which(uvstab$Exposure=="HotQUV"), ]
# uvstab.cq <- uvstab[which(uvstab$Exposure=="CyclicQUV"), ]

# Exposures for UV stabilized

hystab.dh <- filter(hystab, Exposure == "DampHeat")
```

```
hystab.ft <- filter(hystab, Exposure == "FreezeThaw")
hystab.hq <- filter(hystab, Exposure == "HotQUV")
hystab.cq <- filter(hystab, Exposure == "CyclicQUV")
# hystab.dh <- hystab[which(hystab$Exposure=="DampHeat"), ]
# hystab.ft <- hystab[which(hystab$Exposure=="FreezeThaw"), ]
# hystab.hq <- hystab[which(hystab$Exposure=="HotQUV"), ]
# hystab.cq <- hystab[which(hystab$Exposure=="CyclicQUV"), ]
```

5.1.3.8   Simple Plotting with base graphics, "Plot", Function

- Let's plot YI as a function of Time for Unstabilized in DampHeat exposure

```
plot(unstab.dh$Time, unstab.dh$YI)
```
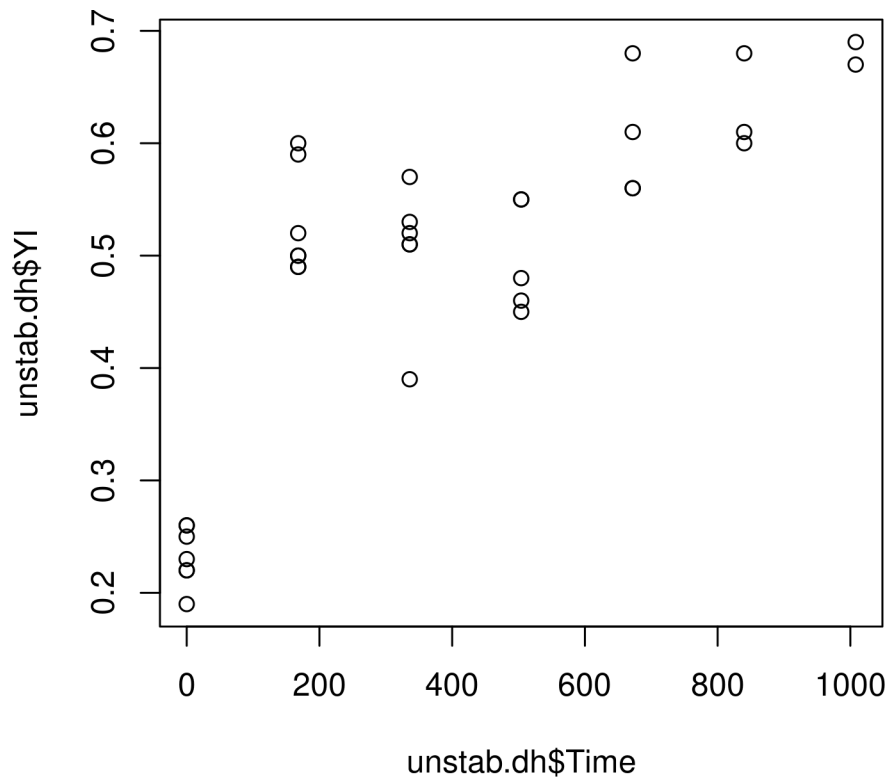


```
plot(
  unstab.dh$Time,
  unstab.dh$YI,
  main = "Change in YI with Time for Unstabilized in
      DampHeat Exposure",
  xlab = "Time(hrs)",
  ylab = "Yellowness Index",
  pch = 19
)
abline(lm(unstab.dh$YI ~ unstab.dh$Time), col = "red")        # Regression line (YI~Time)
```

5.1.3.8.1   Simple Plotting with "Plot" Function

Change in YI with Time for Unstabilized in DampHeat Exposure
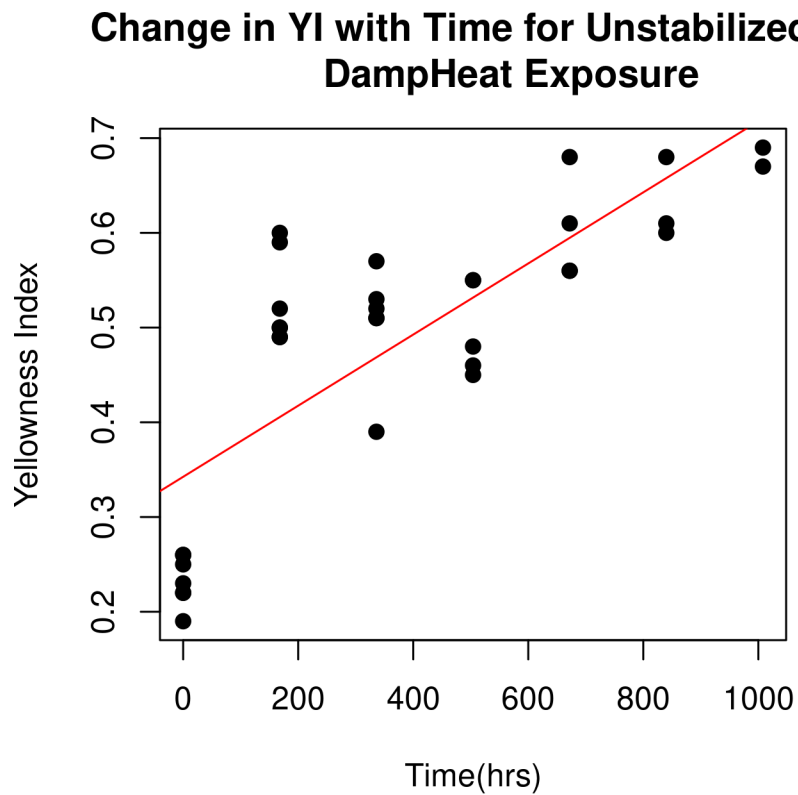
An example of plotting from the main dataframe.

- This is a cleaner way of organizing and plotting data
- as it does not depends on a large number of environmental dataframes.

```
library(ggplot2)

dat %>%
  filter(Material == "Unstab" & Exposure == "DampHeat") %>%
  ggplot(aes(x = Time, y = YI)) +
  geom_point(color = 'red', pch = 19) +
  geom_smooth(method = 'lm', se = FALSE) +
  labs(xlab = "Time(hrs)", ylab = "Yellowness Index", title = "Change in YI with Time for Unstabilized
  theme(plot.title = element_text(size = 10))
```

Change in YI with Time for Unstabilized in DampHeat Exposure
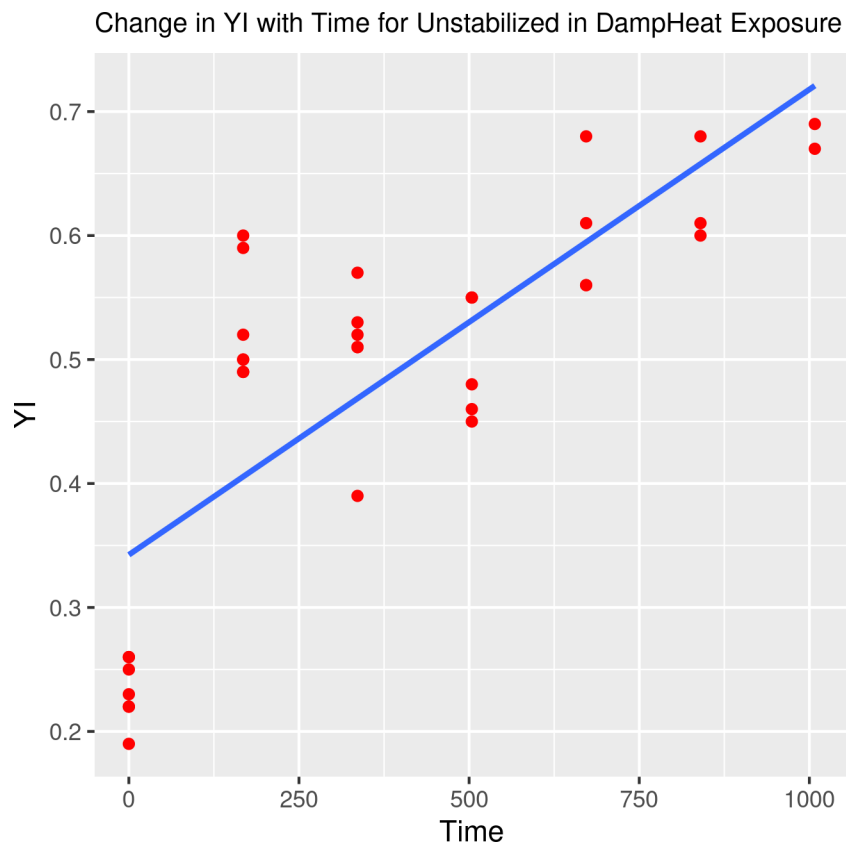
5.1.3.8.2 Simple Plotting with "Plot" Function

- Another example: Plot of haze as a function of Time for Hydstab in CyclicQUV

```
plot(
  hystab.cq$Time,
  hystab.cq$Haze,
  main = "Change in Haze with Time for Hyd. stabilized in CyclicQUV Exposure",
  xlab = "Time(hrs)",
  ylab = "Haze(%)",
  pch = 19,
  col = "red"
)

abline(lm(hystab.cq$Haze ~ hystab.cq$Time), col = "blue")        # Regression line (YI~Time)
```
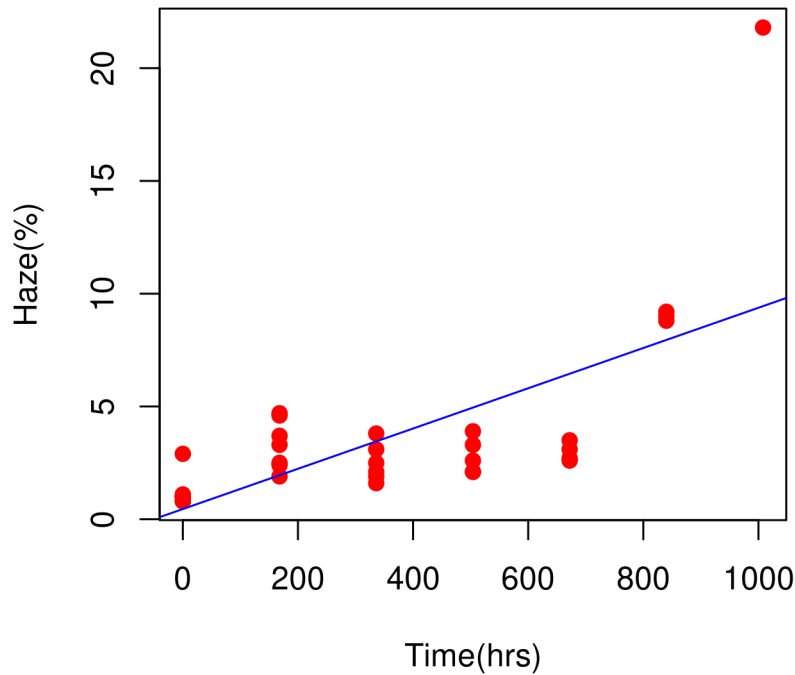
```
pairs( ~ Time + YI + Haze + abs300 + abs400 + iad300 + iad400,
       data = uvstab.hq,
       main = "Pairwise plot for UVstabilized in HotQUV Exposure")
```

5.1.3.9 Pairwise plots

Pairwise plot for UVstabilized in HotQUV Exposure
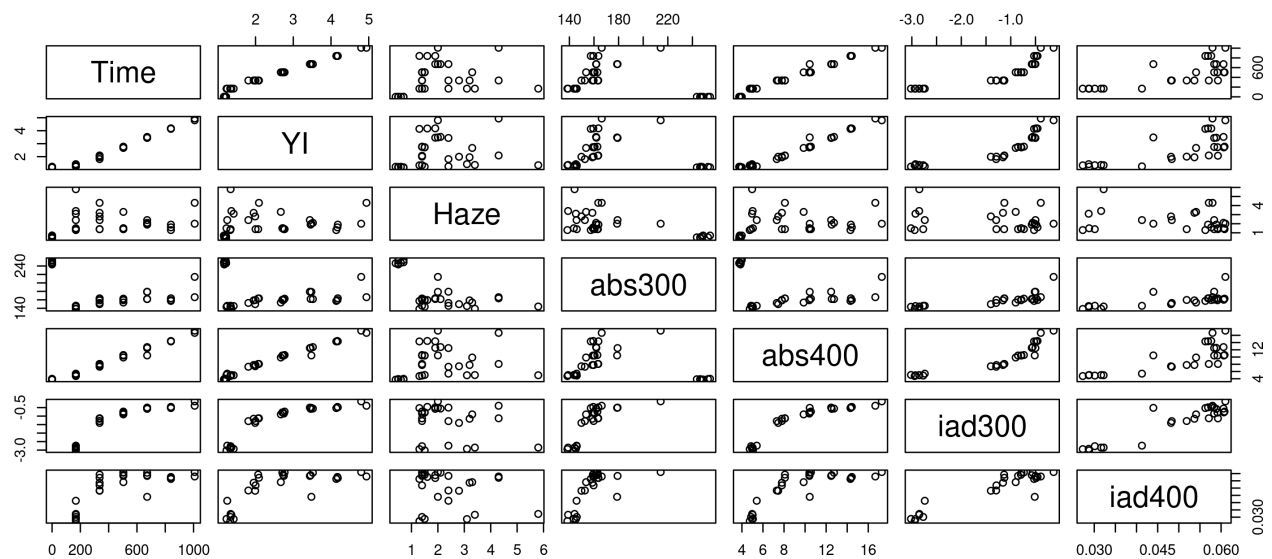

```
ggpairwise <-
  ggpairs(uvstab.hq[, c(6, 13, 14, 15, 20, 21, 26)],
```

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```
              title = "Pairwise plot with correlation coeff's for UVstabilized in HotQUV Exposure")
ggpairwise
```

5.1.3.9.1   Pairwise plots

Pairwise plot with correlation coeff's for UVstabilized in
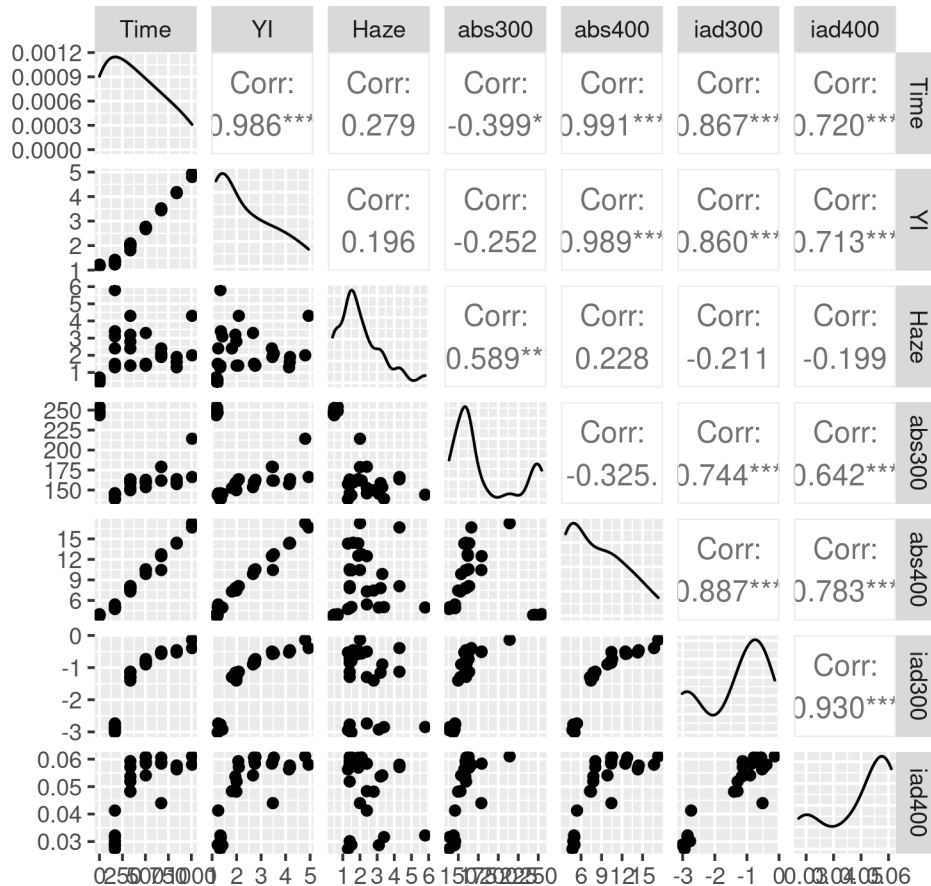
5.1.3.10   Standard deviation, standard error, and 95% confidence interval

- Subsetting data for baseline measurements for each material type

```
# Subset data for time zero

  unstab.0 <- filter(dat, Material == "Unstab" & Time == "0")
  uvstab.0 <- filter(dat, Material == "UVStab" & Time == "0")
  hystab.0 <- filter(dat, Material == "HydStab" & Time == "0")

# unstab.0 <- subset(dat, Material=="Unstab" & Time=="0")
# uvstab.0 <- subset(dat, Material=="UVStab" & Time=="0")
# hystab.0 <- subset(dat, Material=="HydStab" & Time=="0")
```

Just as an example

```
  head(unstab.0)[1:8]
```

```
##                  Rowkey      Sample Material  Thick Exposure Time Step Irrad
## 1 sa19603.00-step0 sa19603.00   Unstab 0.0075 Baseline    0    0    NA
## 2 sa19603.01-step0 sa19603.01   Unstab 0.0075 DampHeat    0    0     0
```

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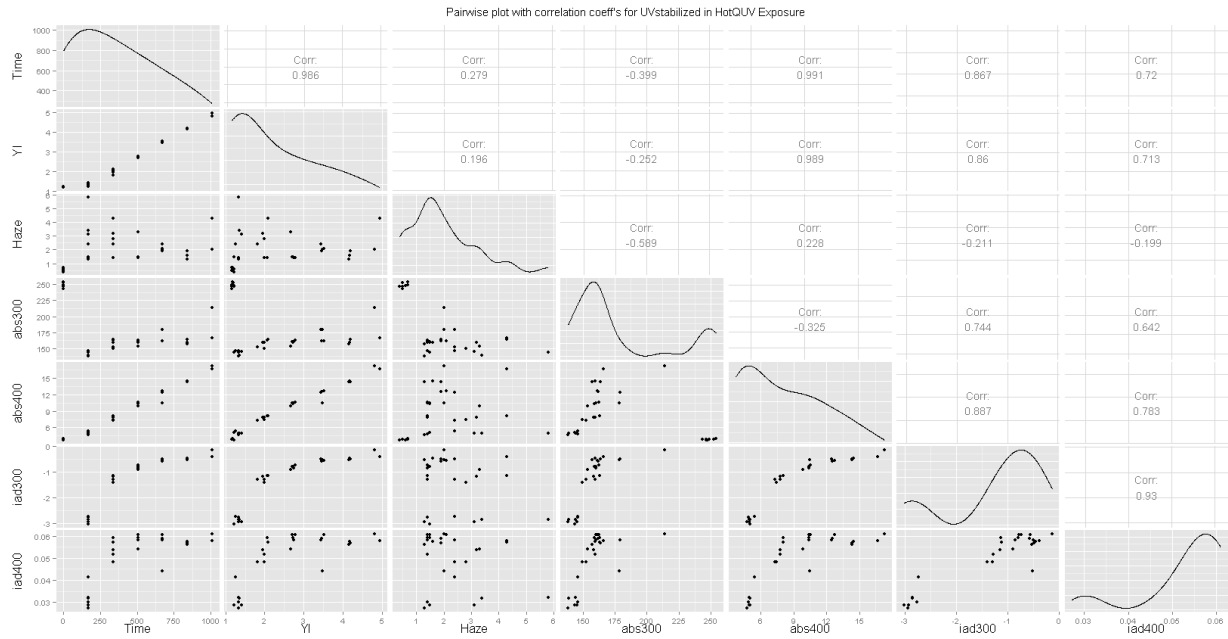
Figure 5: Figure

```
## 3 sa19603.02-step0 sa19603.02   Unstab 0.0075 DampHeat   0    0    0
## 4 sa19603.03-step0 sa19603.03   Unstab 0.0075 DampHeat   0    0    0
## 5 sa19603.04-step0 sa19603.04   Unstab 0.0075 DampHeat   0    0    0
## 6 sa19603.05-step0 sa19603.05   Unstab 0.0075 DampHeat   0    0    0
```

```
glimpse(unstab.0)
```

```
## Rows: 30
## Columns: 34
## $ Rowkey   <chr> "sa19603.00-step0", "sa19603.01-step0", "~
## $ Sample   <chr> "sa19603.00", "sa19603.01", "sa19603.02", "sa19603.03", "sa19~
## $ Material <chr> "Unstab", "Unstab", "Unstab", "Unstab", "Unstab", "Unstab", "~
## $ Thick    <dbl> 0.0075, 0.0075, 0.0075, 0.0075, 0.0075, 0.0075, 0.0075, 0.007~
## $ Exposure <chr> "Baseline", "DampHeat", "DampHeat", "DampHeat", "DampHeat", "~
## $ Time     <int> 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0~
## $ Step     <int> 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0~
## $ Irrad    <dbl> NA, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.0~
## $ Pdose    <dbl> NA, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, ~
## $ L        <dbl> 95.90, 95.77, 95.77, 95.79, 95.75, 95.73, 95.77, 95.74, 95.76~
## $ a        <dbl> -0.06, -0.05, -0.05, -0.05, -0.05, -0.04, -0.04, -0.05, -0.05~
## $ b        <dbl> 0.09, 0.16, 0.15, 0.15, 0.17, 0.14, 0.13, 0.16, 0.15, 0.17, 0~
## $ YI       <dbl> 0.10, 0.26, 0.23, 0.22, 0.26, 0.22, 0.19, 0.25, 0.23, 0.28, 0~
## $ Haze     <dbl> 0.7, 0.7, 0.5, 0.5, 0.5, 0.7, 1.0, 0.5, 0.7, 0.5, 0.5, 0.5, 0~
## $ abs300   <dbl> NA, 191.4218, 197.5940, 194.4407, 199.5686, 200.0952, 196.745~
## $ abs335   <dbl> NA, 3.983921, 3.807277, 3.955309, 4.053765, 3.838366, 4.04018~
## $ abs345   <dbl> NA, 2.767227, 2.462322, 2.440824, 2.700257, 2.453022, 2.64619~
## $ abs350   <dbl> NA, 2.181735, 2.060797, 2.058183, 2.223009, 2.138228, 2.16300~
## $ abs370   <dbl> NA, 0.9192707, 0.7923671, 0.8242304, 0.9953029, 0.8507452, 0.~
## $ abs400   <dbl> NA, 0.048536744, -0.029379267, -0.087693770, 0.030005735, 0.0~
## $ iad300   <dbl> NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, N~
## $ iad335   <dbl> NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, N~
```

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```
## $ iad345   <dbl> NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, N~
## $ iad350   <dbl> NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, N~
## $ iad370   <dbl> NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, N~
## $ iad400   <dbl> NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, N~
## $ ftir1716 <dbl> NA, 0.3100746, 0.6101339, 0.6349439, 0.6540887, 0.5419867, 0.~
## $ ftir1409 <dbl> NA, 0.1226776, 0.1902809, 0.1949499, 0.1980377, 0.1394507, 0.~
## $ ftir1341 <dbl> NA, 0.1451086, 0.2257809, 0.2304419, 0.2349576, 0.1957127, 0.~
## $ ftir1251 <dbl> NA, 0.3477596, 0.6651109, 0.6851199, 0.7029827, 0.5619947, 0.~
## $ ftir1093 <dbl> NA, 0.3451416, 0.6140299, 0.6284049, 0.6431516, 0.5635907, 0.~
## $ ftir1017 <dbl> NA, 0.2610076, 0.4055479, 0.4103479, 0.4168606, 0.4004427, 0.~
## $ ftir872  <dbl> NA, 0.2792076, 0.4359609, 0.4407899, 0.4481156, 0.4594207, 0.~
## $ ftir714  <dbl> NA, 0.5304336, 0.9366959, 0.9465499, 0.9635357, 0.8771207, 0.~
```

5.1.3.10.1 Standard deviation, standard error, and 95% confidence interval

- For yellowness index measurement for each material

```
library(Rmisc)
```

```
## Loading required package: lattice
```

```
## Loading required package: plyr
```

```
## ------------------------------------------------------------------------------
```

```
## You have loaded plyr after dplyr - this is likely to cause problems.
## If you need functions from both plyr and dplyr, please load plyr first, then dplyr:
## library(plyr); library(dplyr)
```

```
## ------------------------------------------------------------------------------
```

```
##
## Attaching package: 'plyr'
```

```
## The following objects are masked from 'package:dplyr':
##
##     arrange, count, desc, failwith, id, mutate, rename, summarise,
##     summarize
```

```
## The following object is masked from 'package:purrr':
##
##     compact
```

```r
# For YI at Time=0 for unstabilized
unstab.yi.unc <-
  summarySE(unstab.0, measurevar = "YI", groupvars = "Time")
print(unstab.yi.unc)
```

```
##   Time  N    YI         sd          se          ci
## 1    0 30 0.248 0.05074616 0.009264938 0.01894893
```

```r
# For YI at Time=0 for UVstabilized
uvstab.yi.unc <-
  summarySE(uvstab.0, measurevar = "YI", groupvars = "Time")
print(uvstab.yi.unc)
```

```
##   Time  N       YI         sd         se          ci
## 1    0 30 1.160333 0.05756456 0.0105098 0.02149496
```

```r
# For YI at Time=0 for Hyd.stabilized
hystab.yi.unc <-
```

```
  summarySE(hystab.0, measurevar = "YI", groupvars = "Time")
print(hystab.yi.unc)
```

```
##   Time  N       YI        sd          se          ci
## 1    0 30 1.430667 0.03204881 0.005851286 0.01196722
```

5.1.3.10.2 Standard deviation, standard error, and 95% confidence interval

- For haze measurement for each material

```
# For Haze at Time=0 for unstabilized
unstab.haze.unc <-
  summarySE(unstab.0, measurevar = "Haze", groupvars = "Time")
print(unstab.haze.unc)
```

```
##   Time  N      Haze        sd         se          ci
## 1    0 30 0.5566667 0.1278019 0.02333333 0.04772202
```

```
# For Haze at Time=0 for UVstabilized
uvstab.haze.unc <-
  summarySE(uvstab.0, measurevar = "Haze", groupvars = "Time")
print(uvstab.haze.unc)
```

```
##   Time  N      Haze        sd         se          ci
## 1    0 30 0.5766667 0.1165106 0.02127182 0.04350576
```

```
# For Haze at Time=0 for Hyd.stabilized
hystab.haze.unc <-
  summarySE(hystab.0, measurevar = "Haze", groupvars = "Time")
print(hystab.haze.unc)
```

```
##   Time  N Haze       sd        se         ci
## 1    0 30 1.33 0.692895 0.1265047 0.2587312
```

```
ggplot(dat, aes(x = Time, y = YI, group = Sample)) + geom_point(alpha = 0.75) +
  geom_line(alpha = 0.75) + facet_grid(Material ~ Exposure) +
  ggtitle("YI: Crossed panels, fixed scale")
```

5.1.3.11 Exploratory Data Analysis

YI: Crossed panels, fixed scale
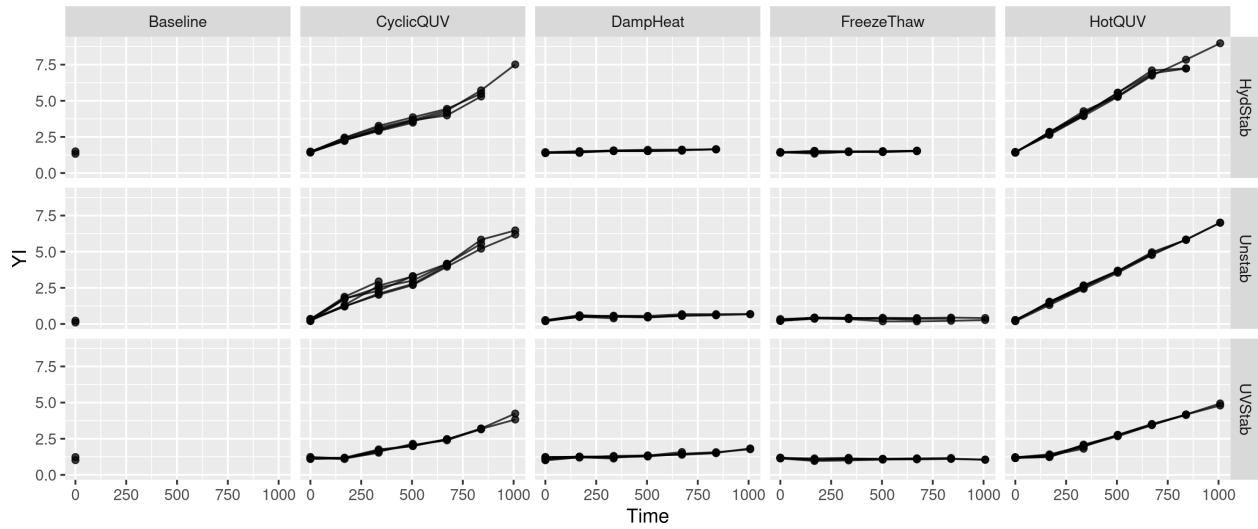

```
ggplot(dat, aes(x = Time, y = Haze, group = Sample)) +
  geom_point(alpha = 0.75, na.rm = FALSE) +
  geom_line(alpha = 0.75) +
  facet_grid(Material ~ Exposure) +
  ggtitle("Haze: Crossed panels, fixed scale")
```

5.1.3.11.1 Exploratory Data Analysis

Haze: Crossed panels, fixed scale
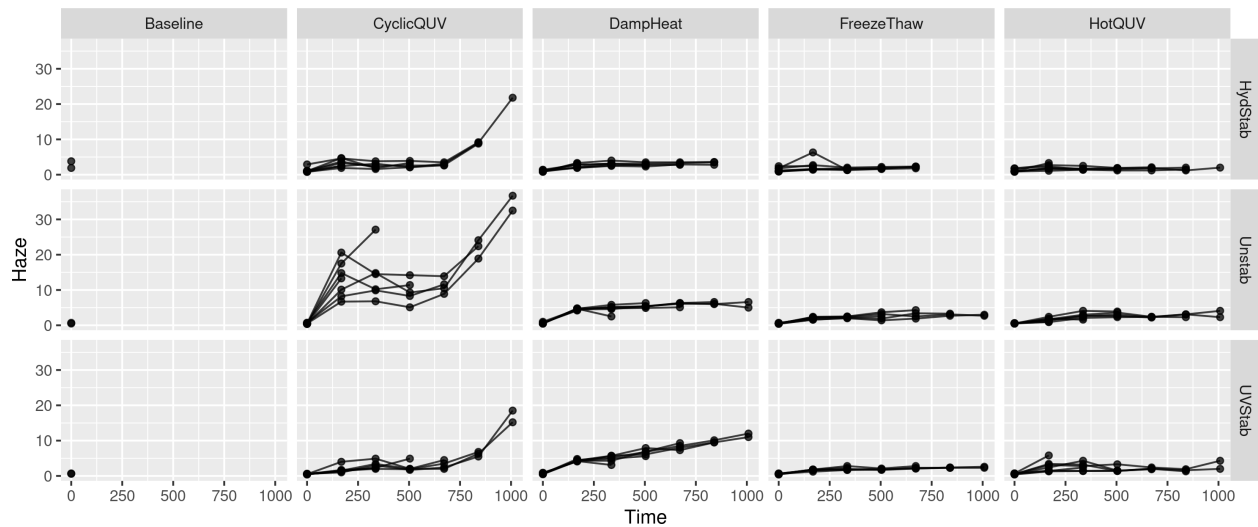
5.1.3.12 Exploratory Data Analysis

5.1.3.13 Exploratory Data Analysis

5.1.3.14 Comments

- Very useful to
  - identify outliers
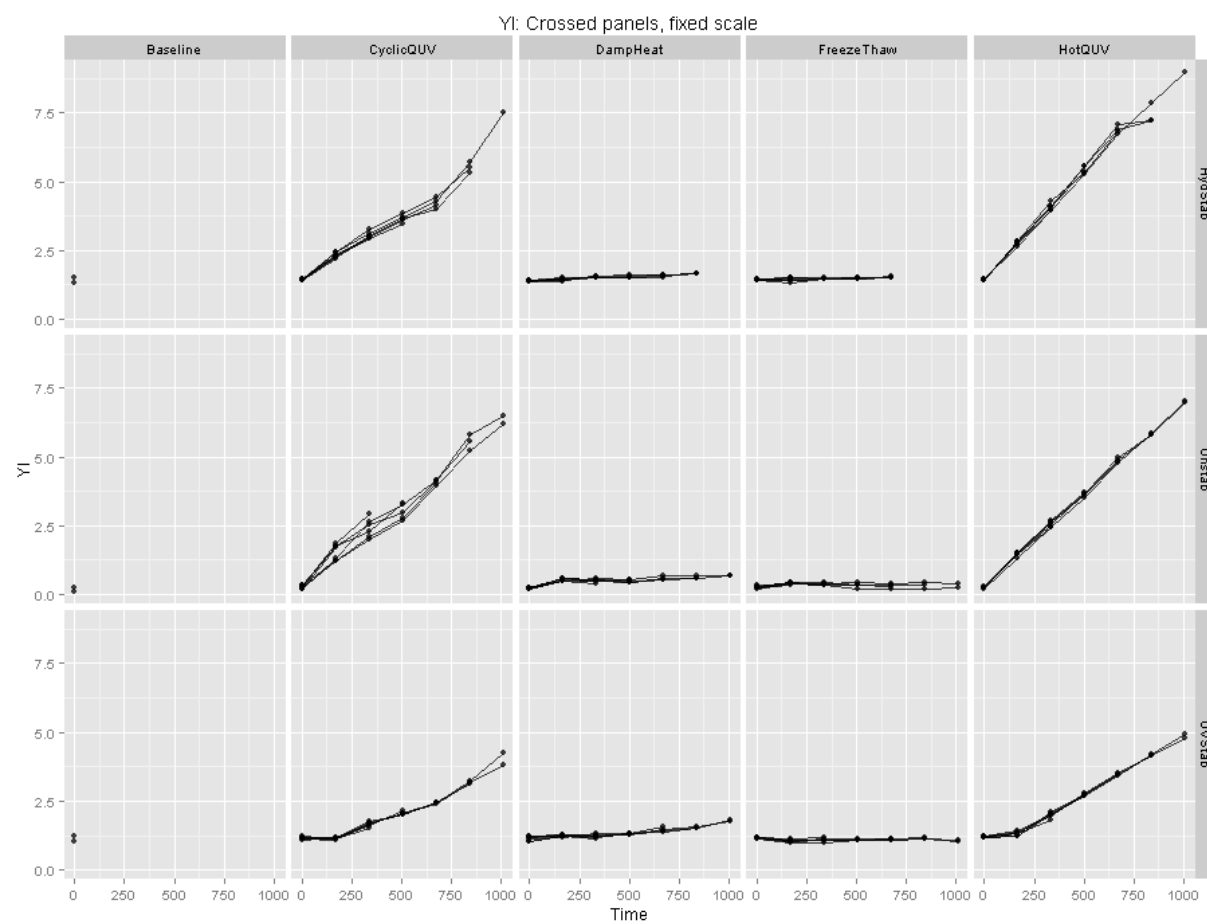
Figure 6: Figure
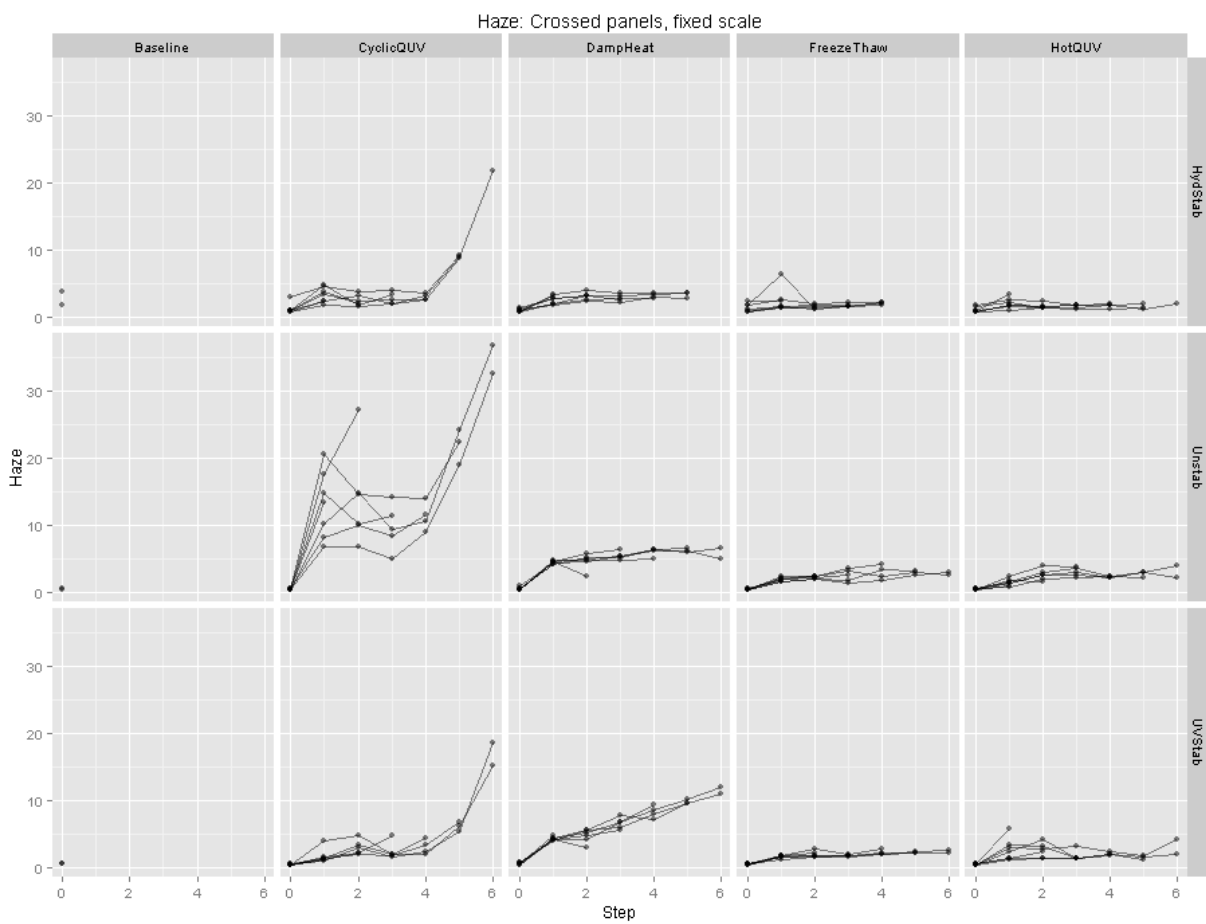
Figure 7: Figure

– Look for trends and change points
  – compare different materials and exposures
  – Observe sample and measurement variability

5.1.3.15   Exploratory Data Analysis

- Absorbance at 300 nm and 400 nm for Unstabilized PET
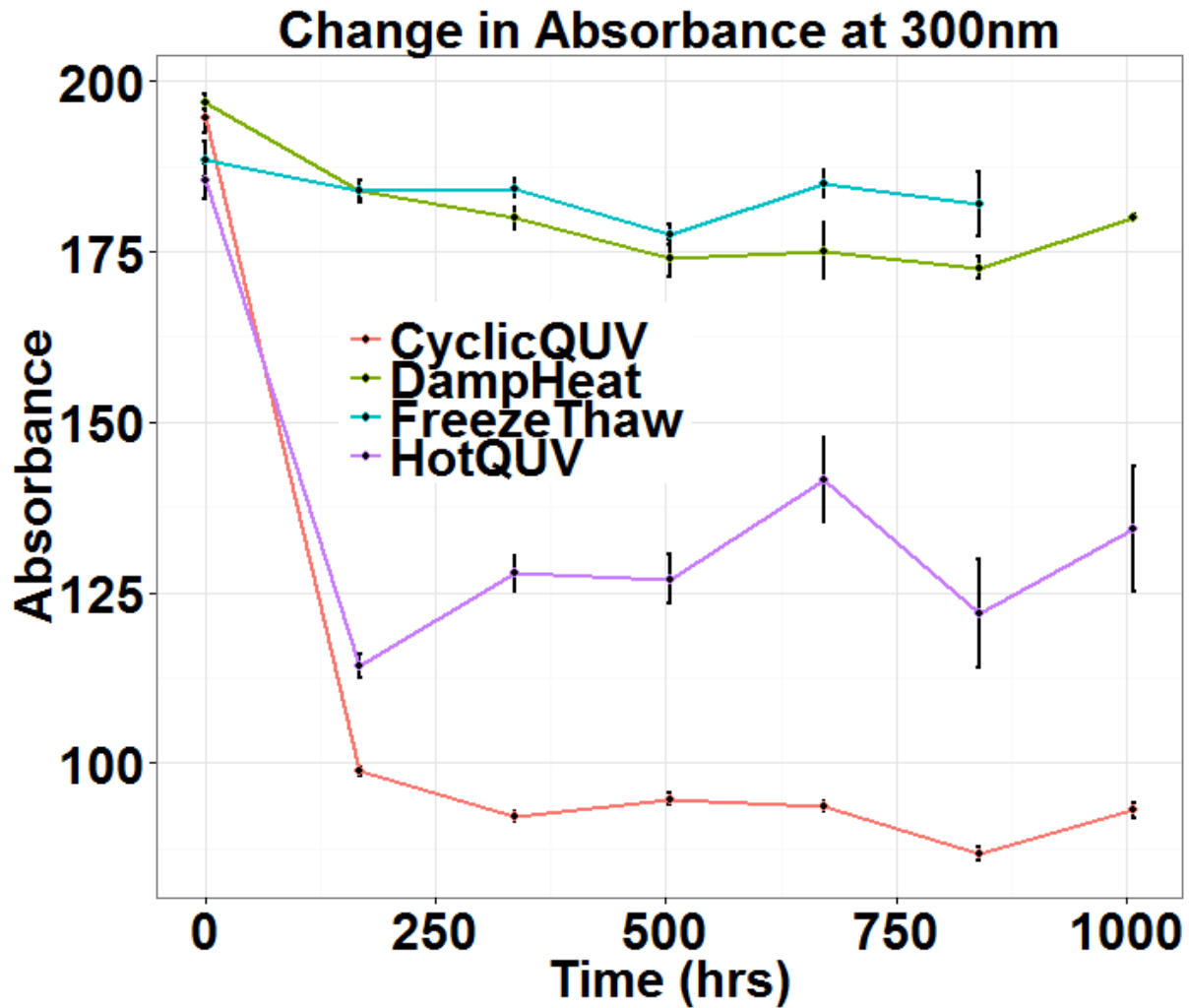
Figure 8: Figure

5.1.3.15.1   Exploratory Data Analysis: IAD of Unstabilized PET

- IAD at 300 nm and 400 nm for Unstabilized PET

5.1.3.15.2   Exploratory Data Analysis: YI and $Haze$

- Yellowness Index and Haze(%) for Unstabilized PET

5.1.3.15.3   Exploratory Data Analysis: Optical Absorbance

- Absorbance at 300 nm and 400 nm for UV stabilized PET
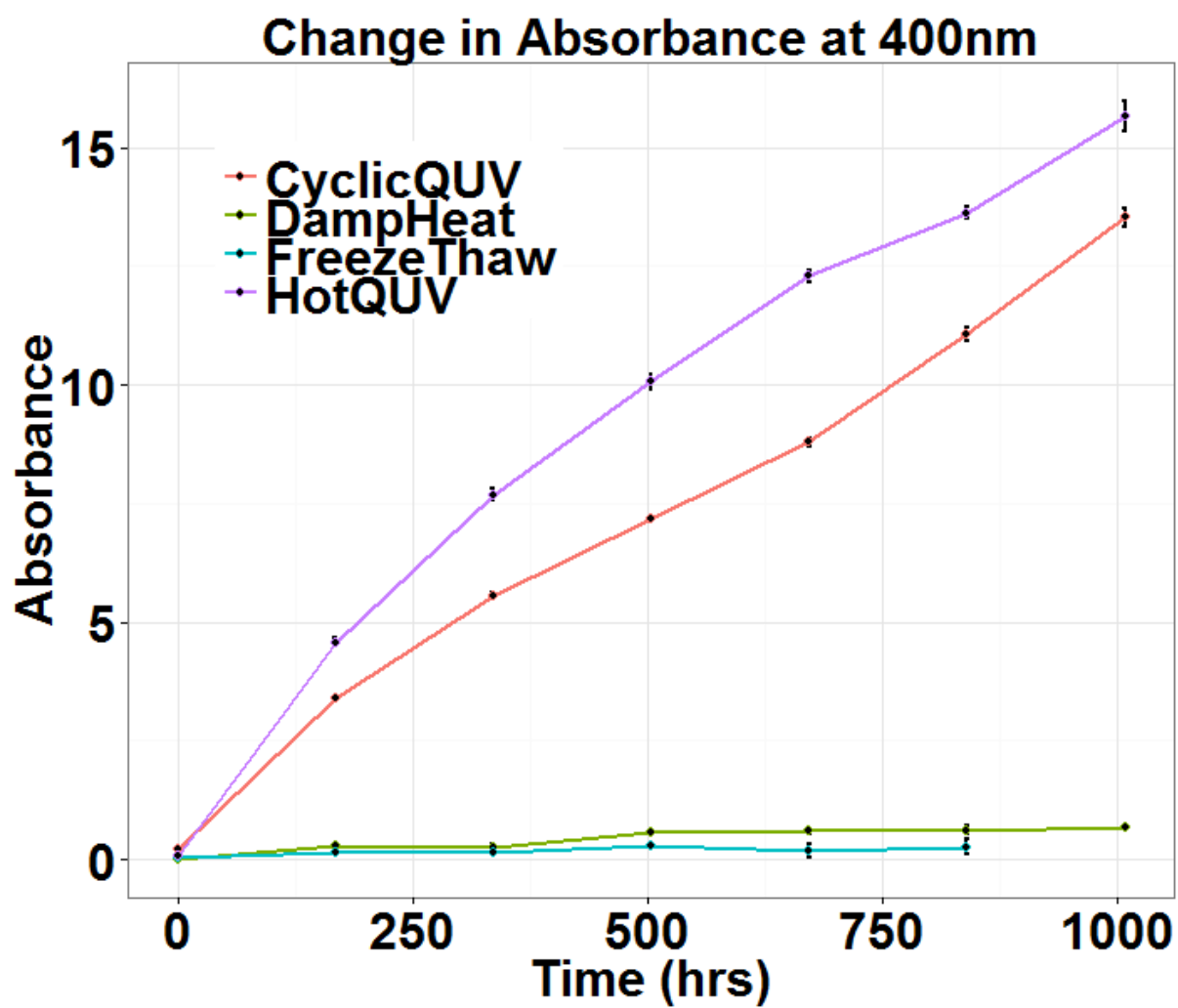
Figure 9: Figure
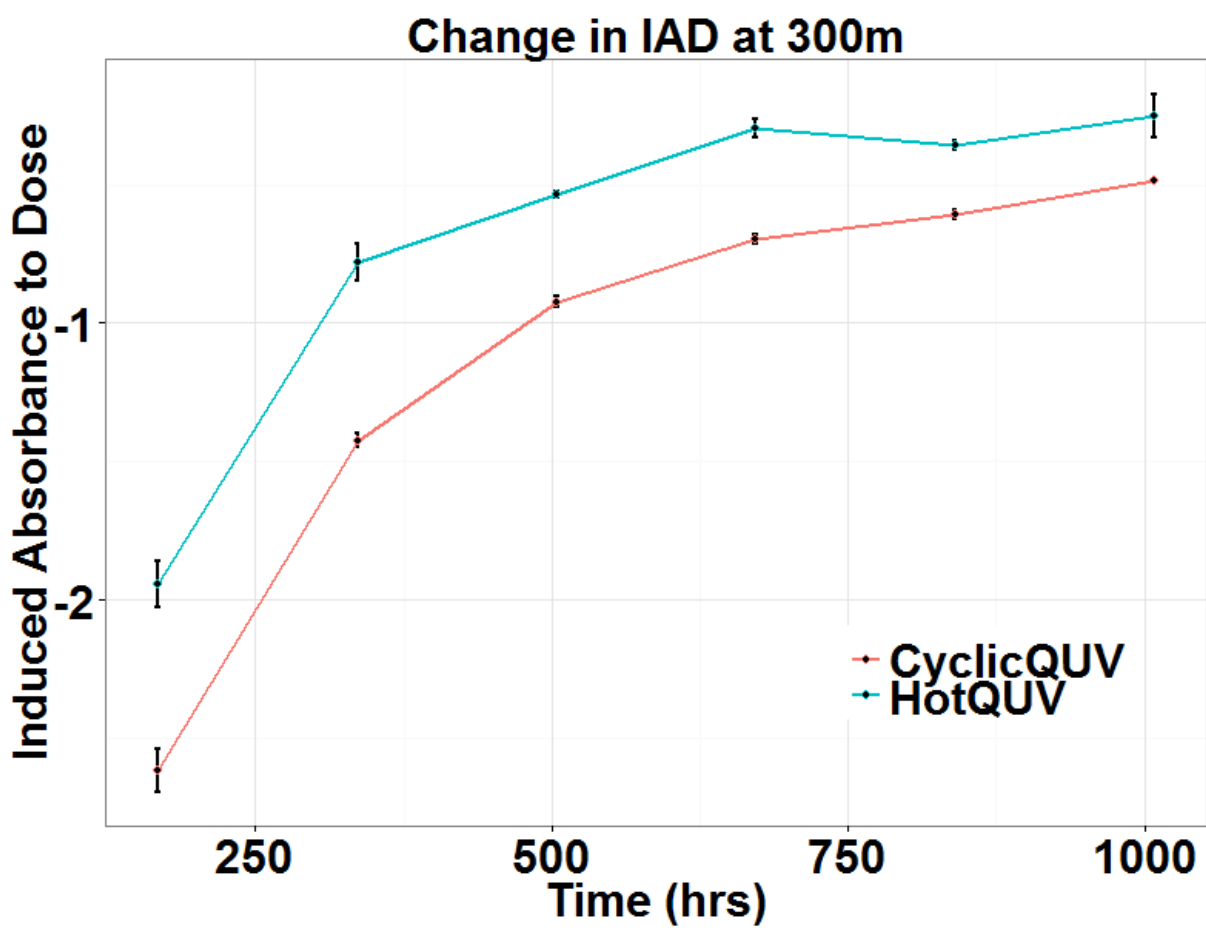
Figure 10: Figure
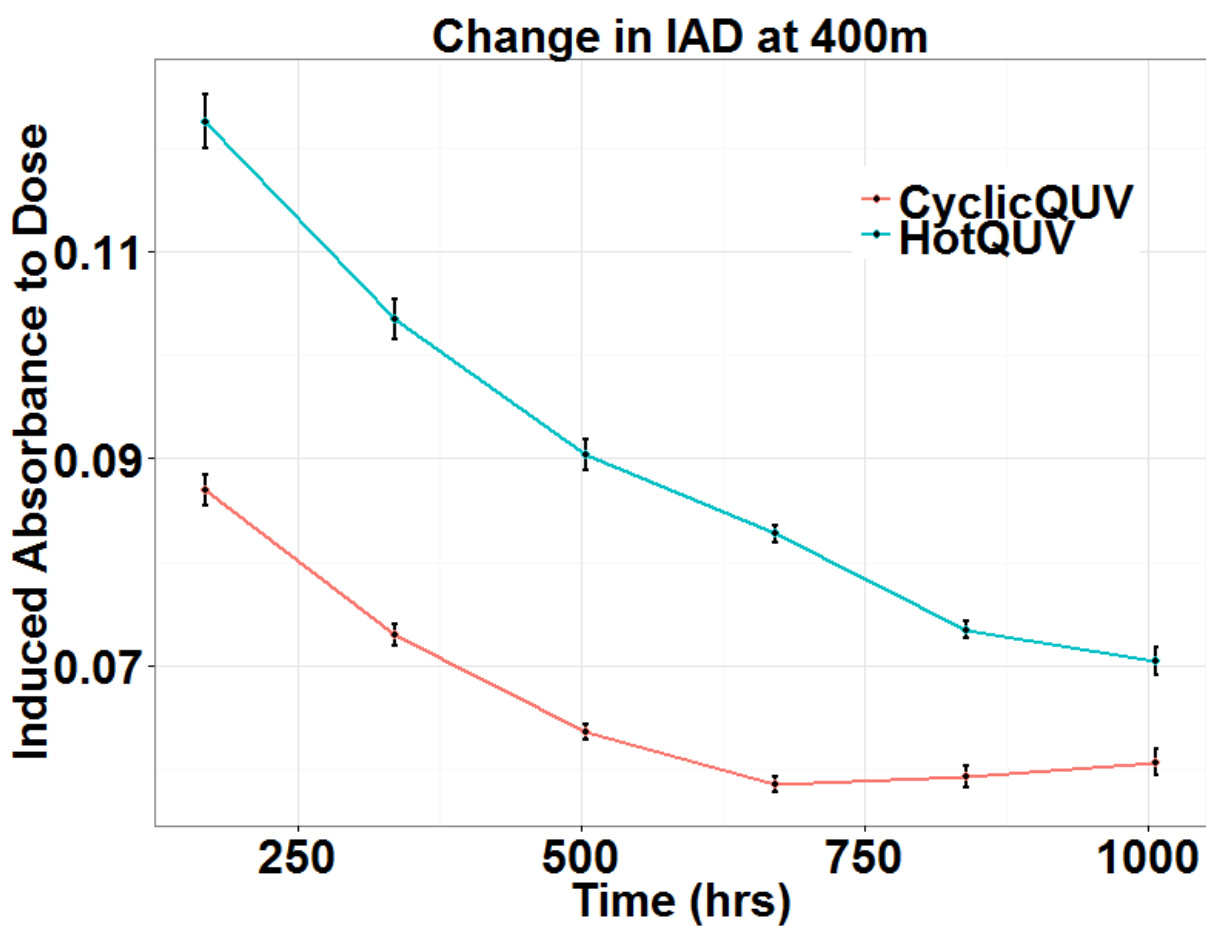
Figure 11: Figure
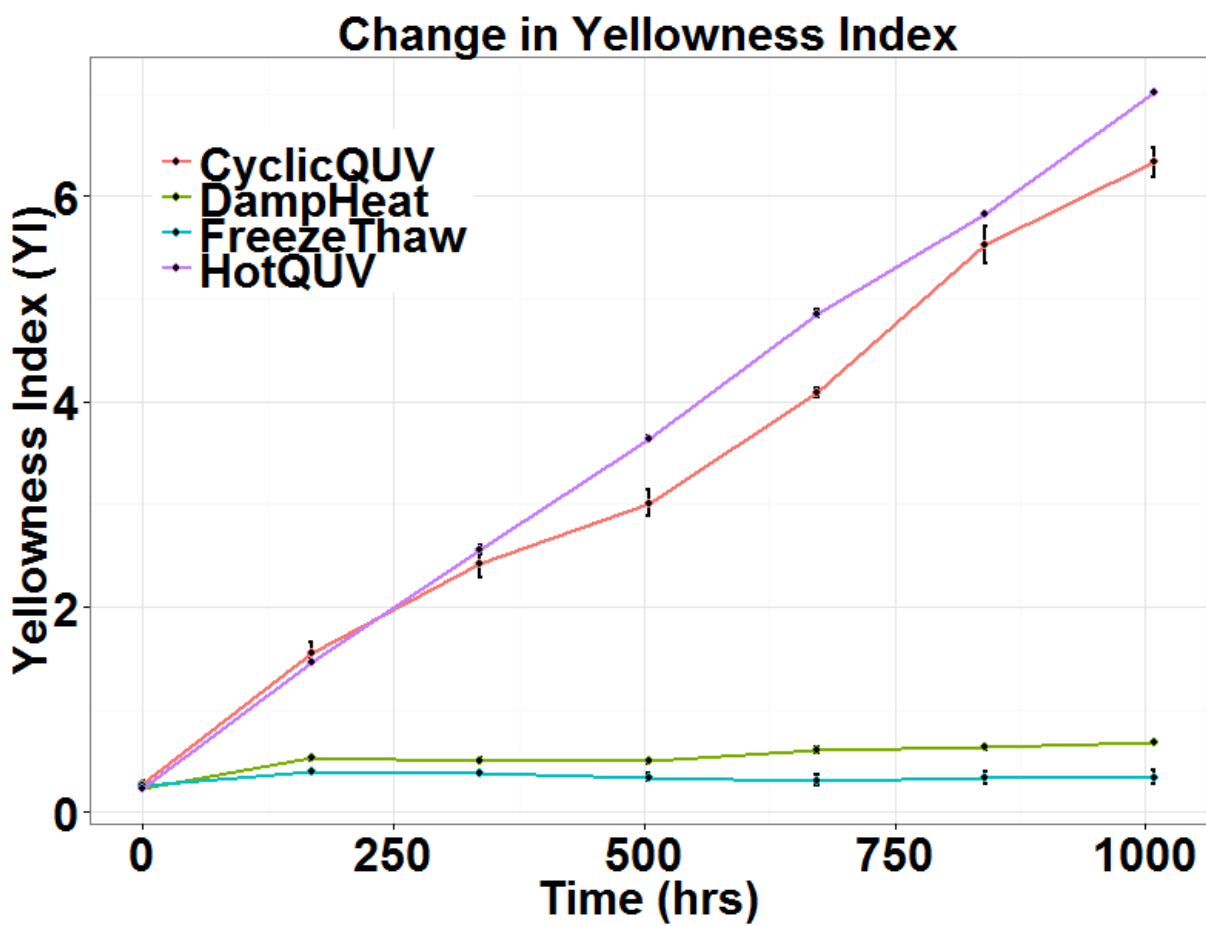
Figure 12: Figure
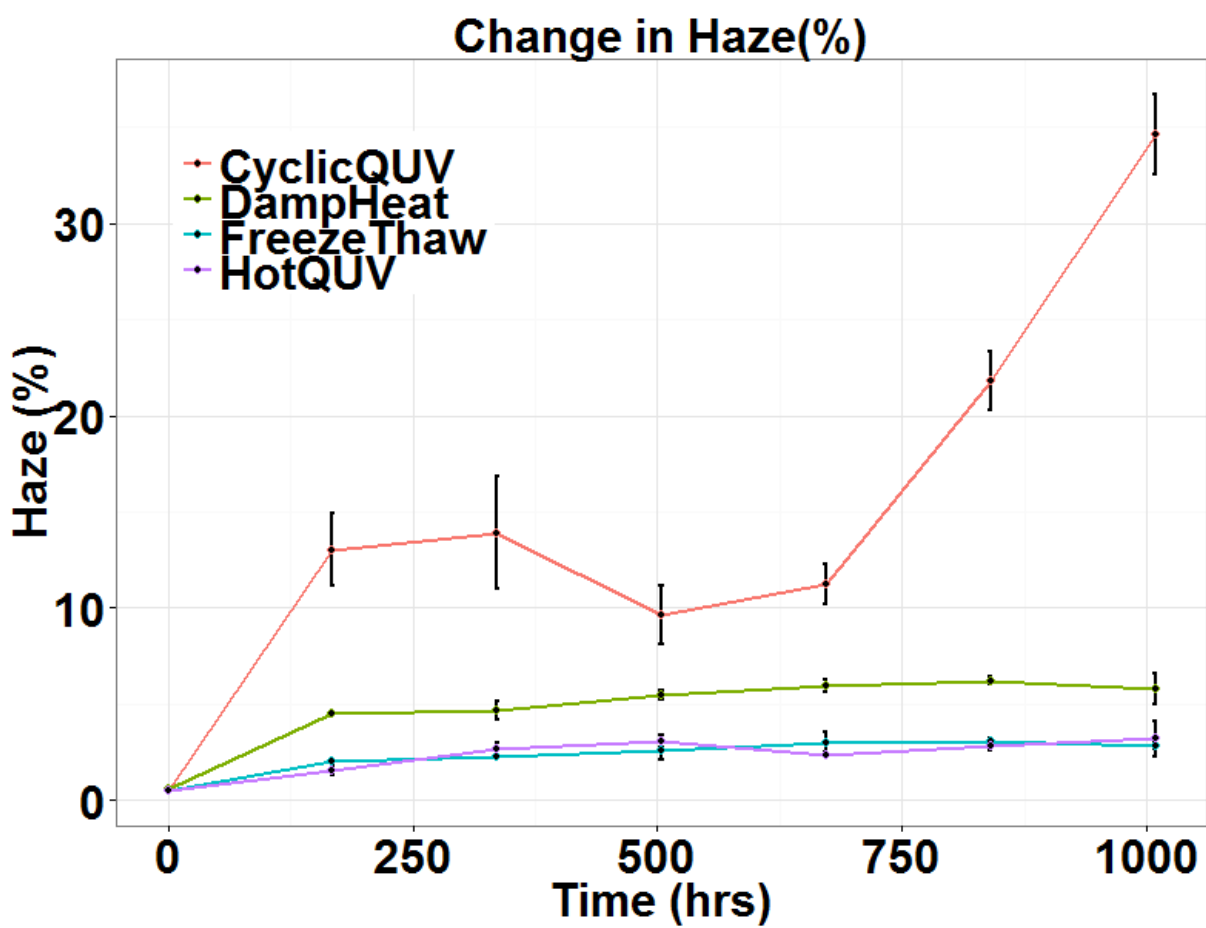
Figure 13: Figure
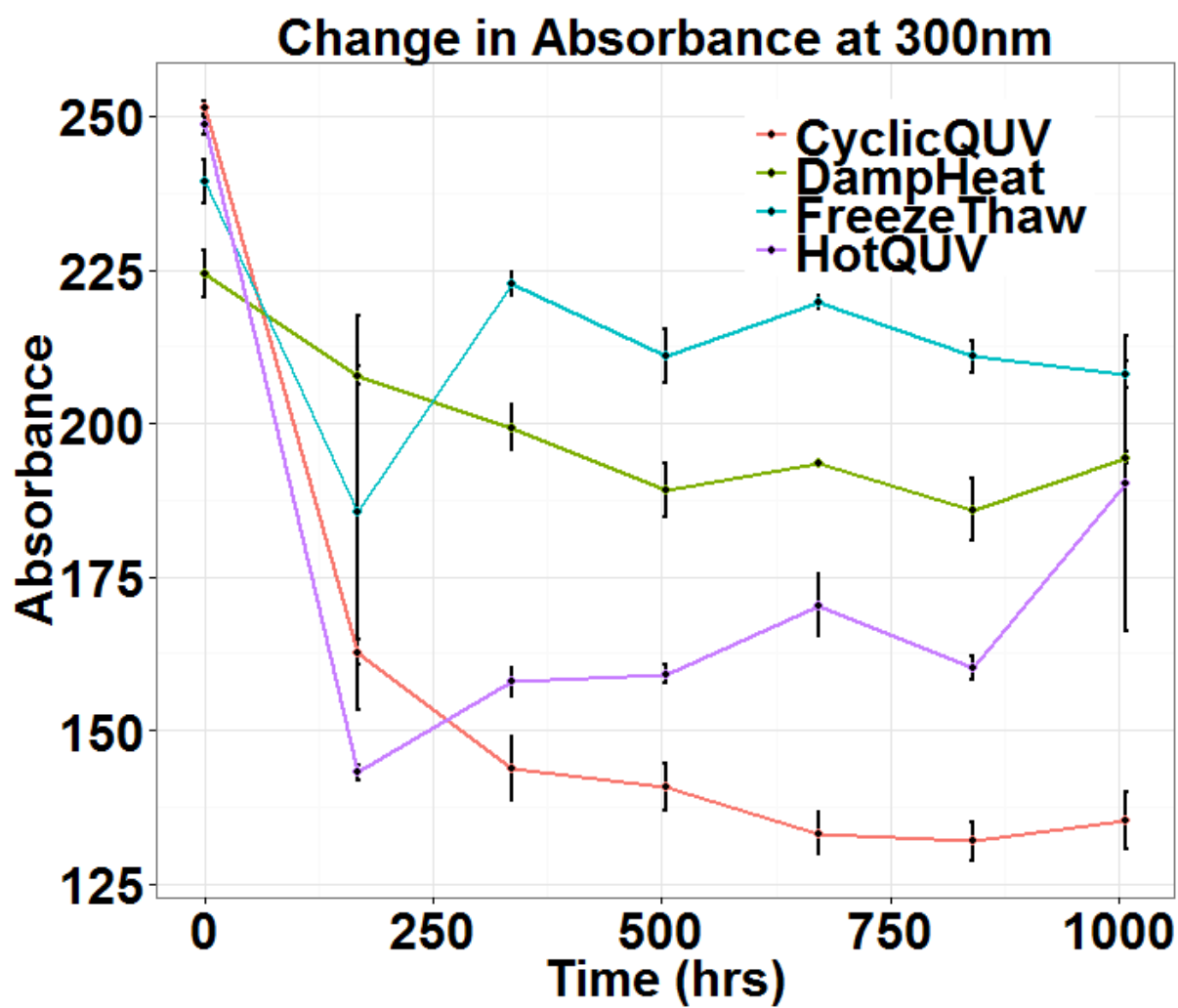
Figure 14: Figure
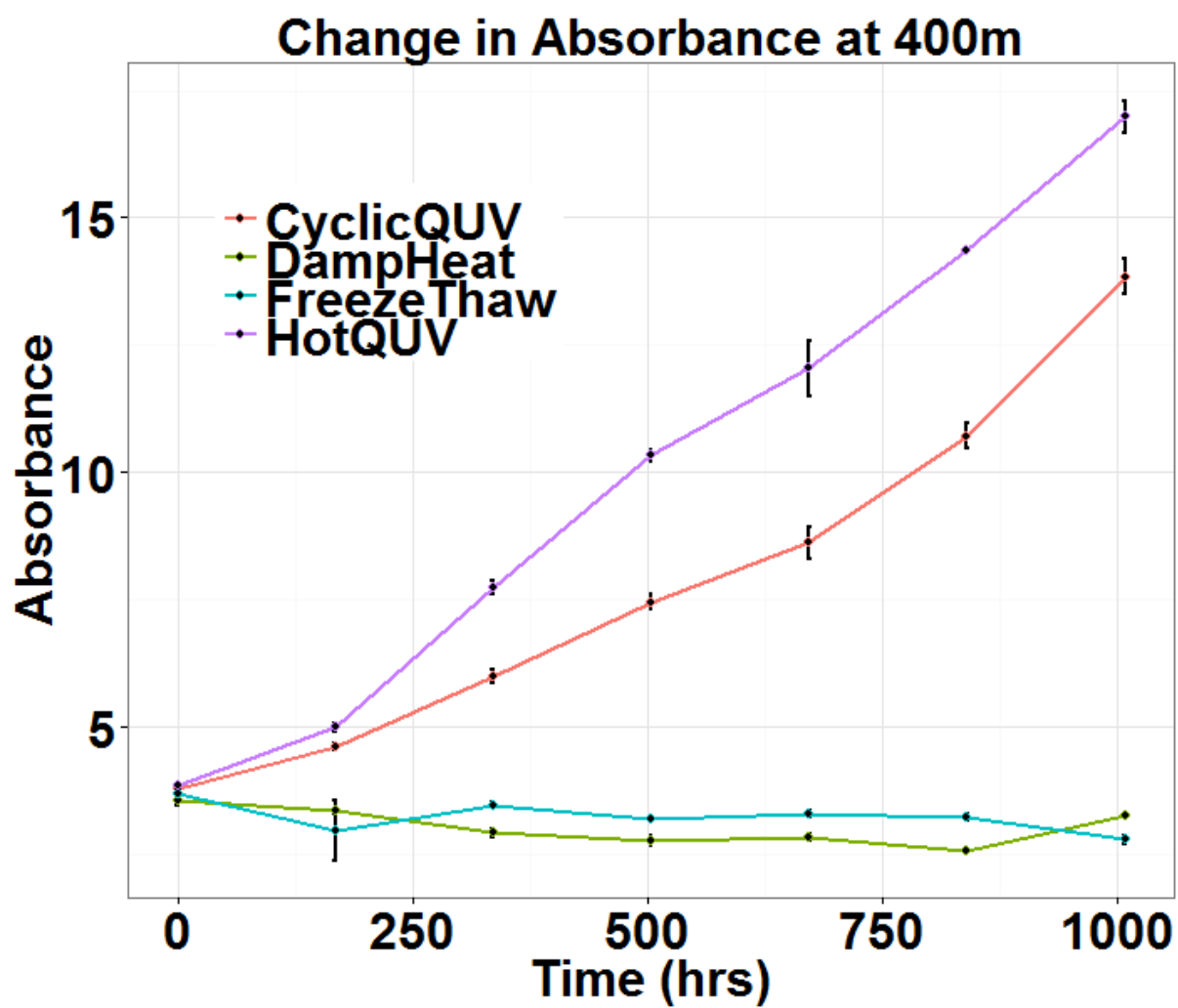
Figure 15: Figure

5.1.3.15.4 Exploratory Data Analysis: IAD UV Stabilized PET

- IAD at 300 nm and 400 nm for UV stabilized PET
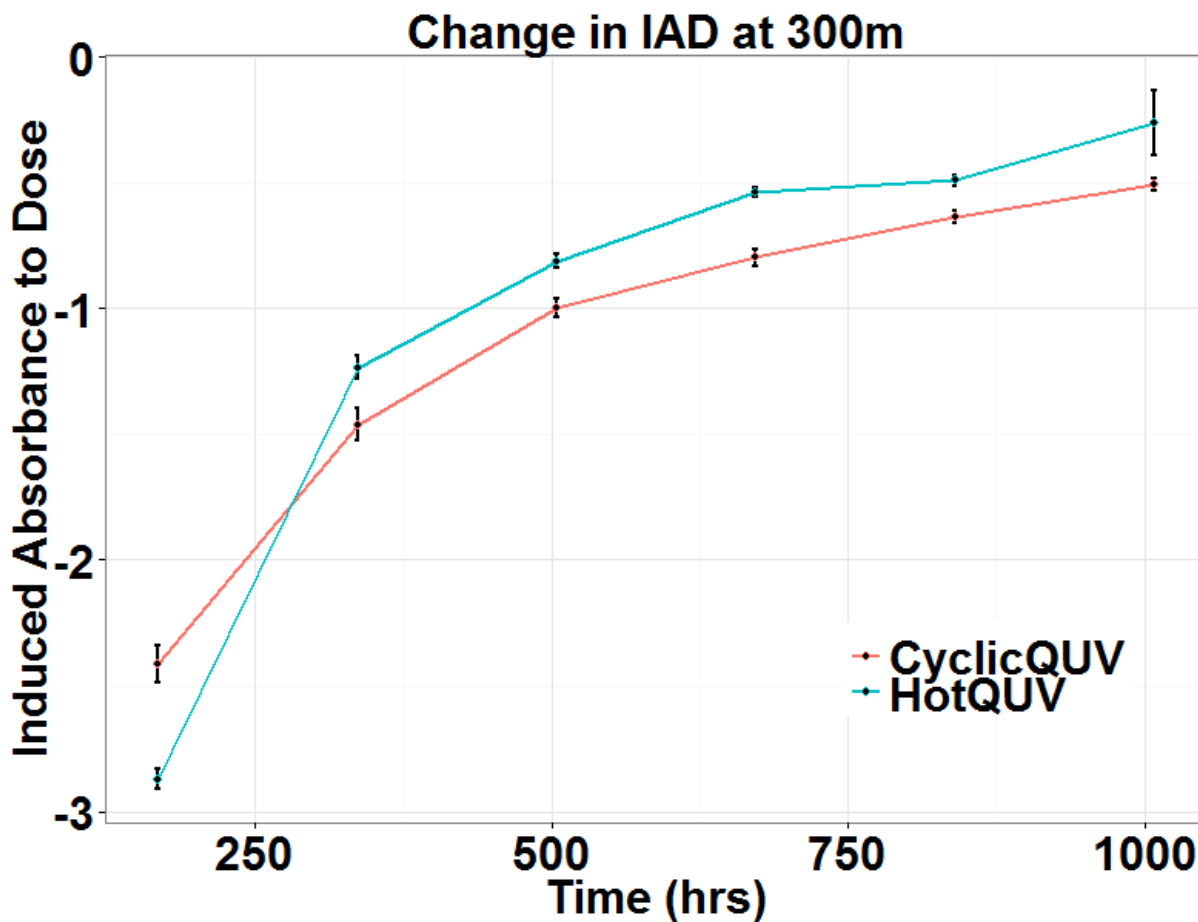
Figure 16: Figure

5.1.3.15.5 Exploratory Data Analysis: YI and $Haze$

- Yellowness Index and Haze(%) for UV stabilized PET

  [Figure](../2-class/figs/UVStab-Haze.png

5.1.3.15.6 Exploratory Data Analysis: Optical Absorbance

- Absorbance at 300 nm and 400 nm for Hyd. stabilized PET

5.1.3.15.7 Exploratory Data Analysis: IAD of Hyd. Stabilized PET

- IAD at 300 nm and 400 nm for Hyd. stabilized PET

5.1.3.15.8 Exploratory Data Analysis: YI and $Haze$

- Yellowness Index and Haze(%) for Hyd. stabilized PET
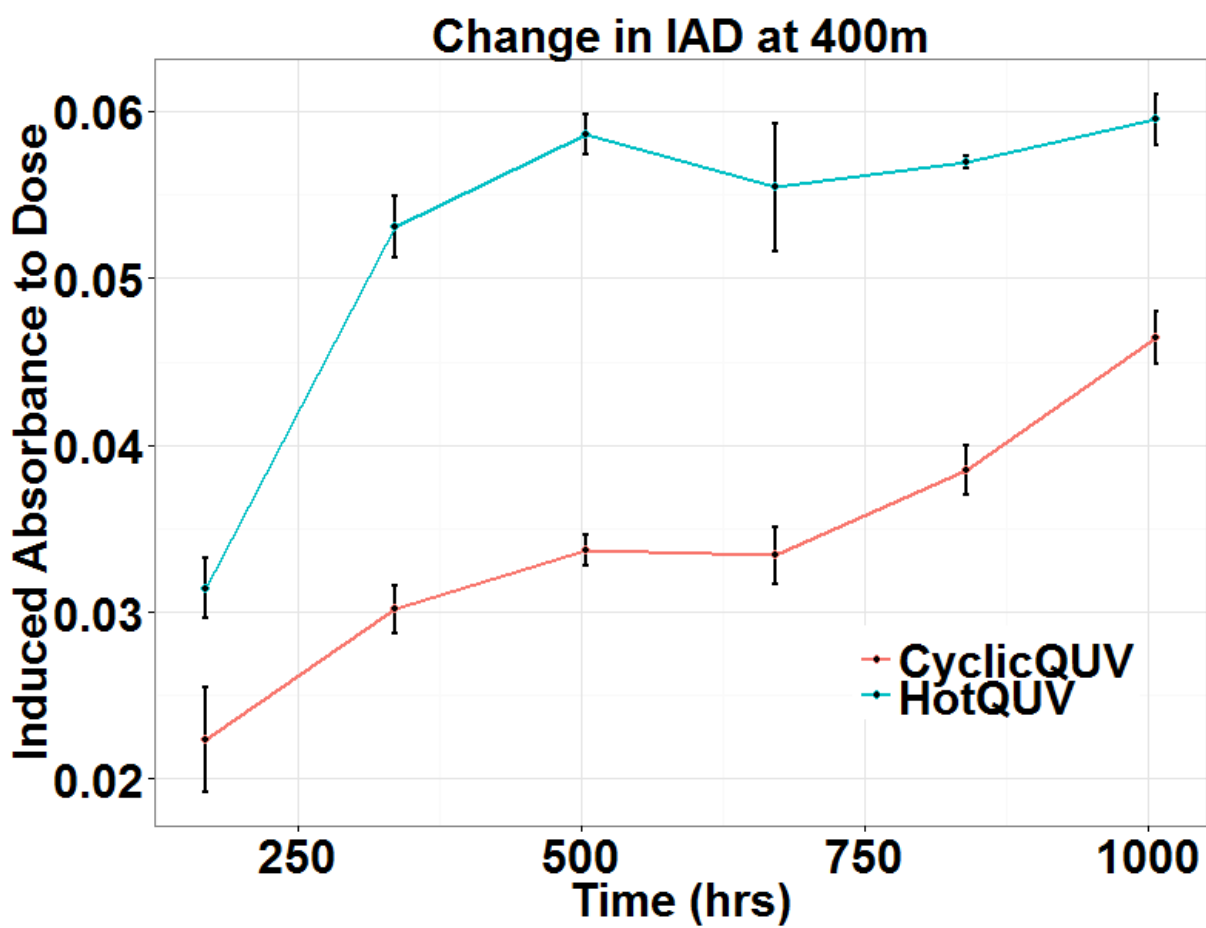
Figure 17: Figure
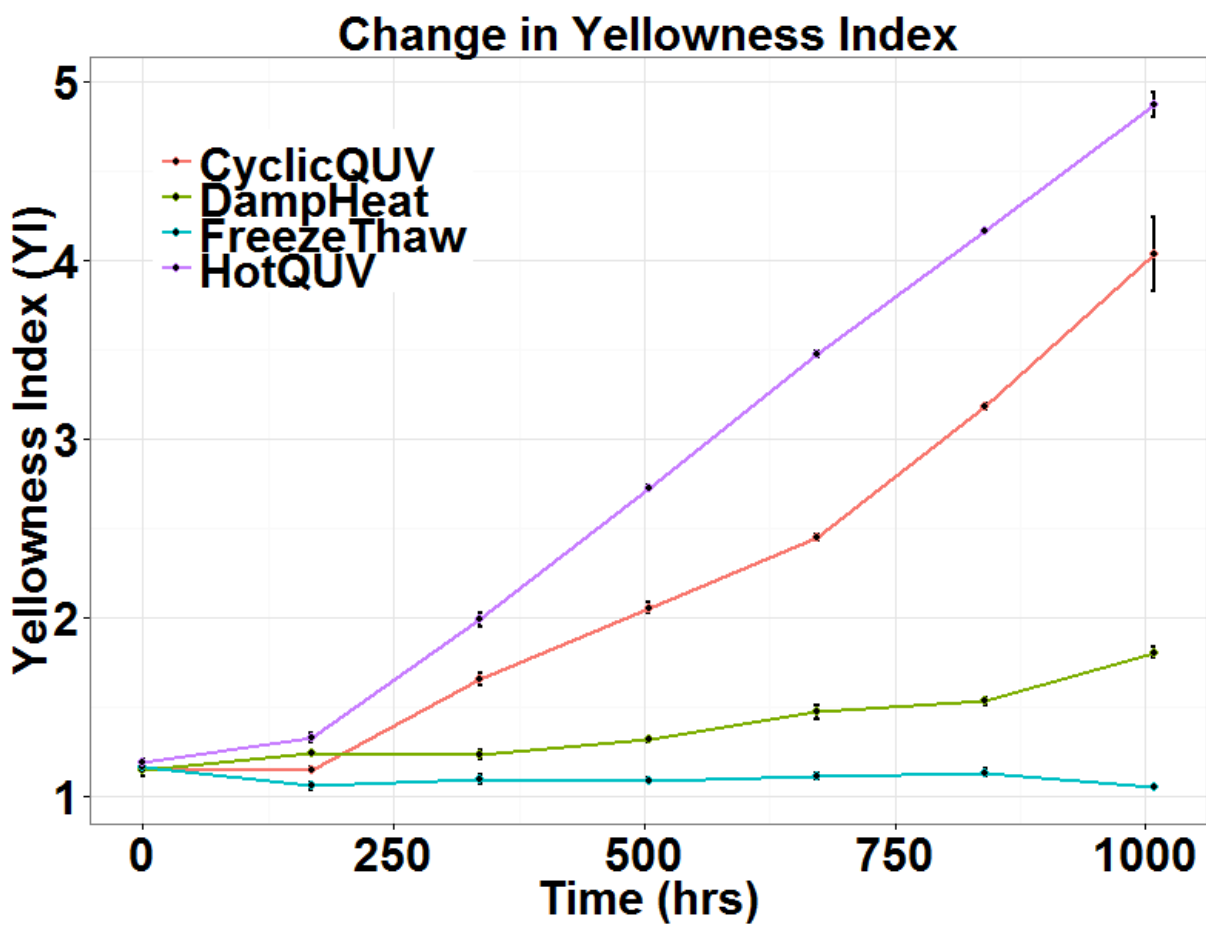
Figure 18: Figure
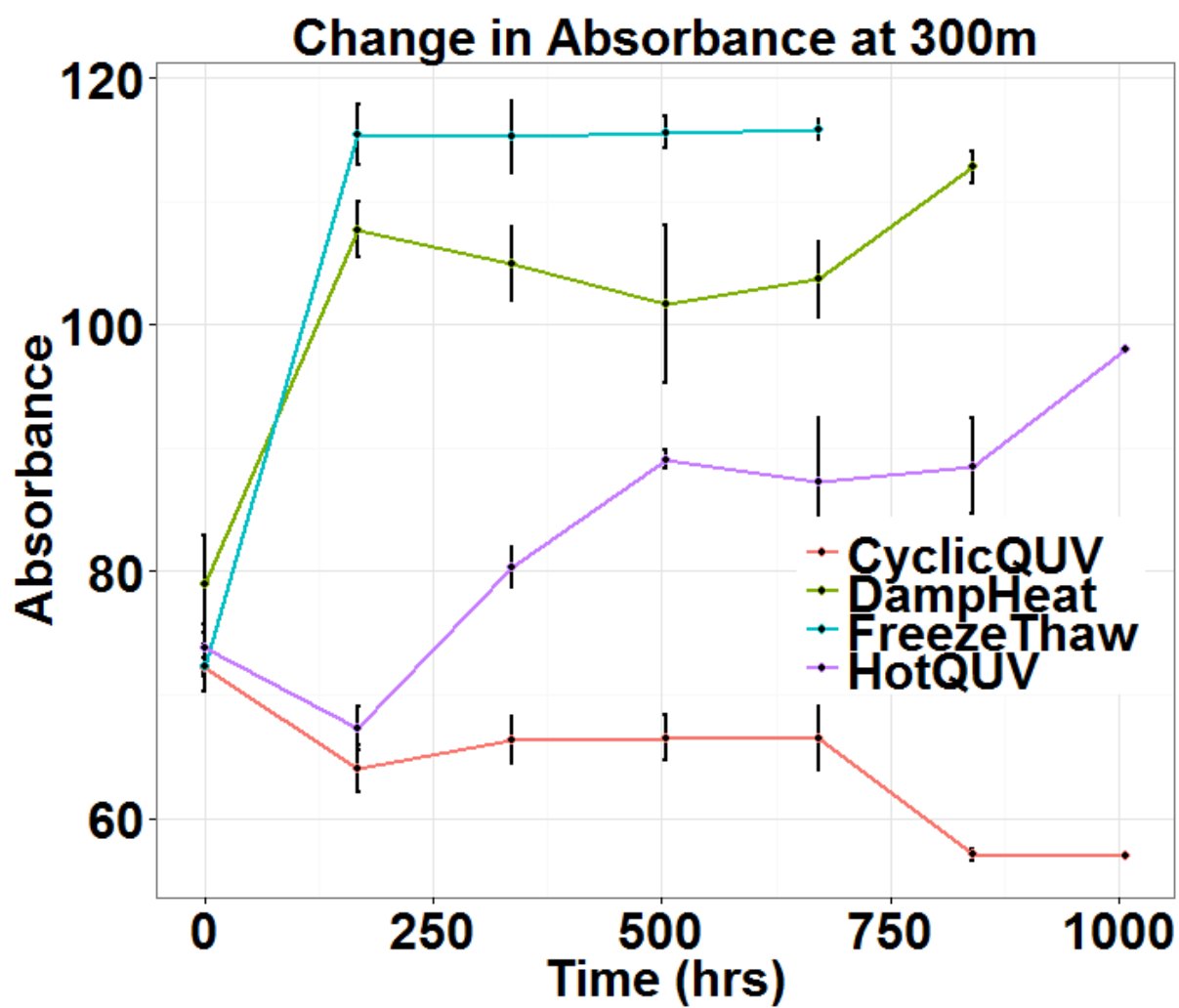
Figure 19: Figure
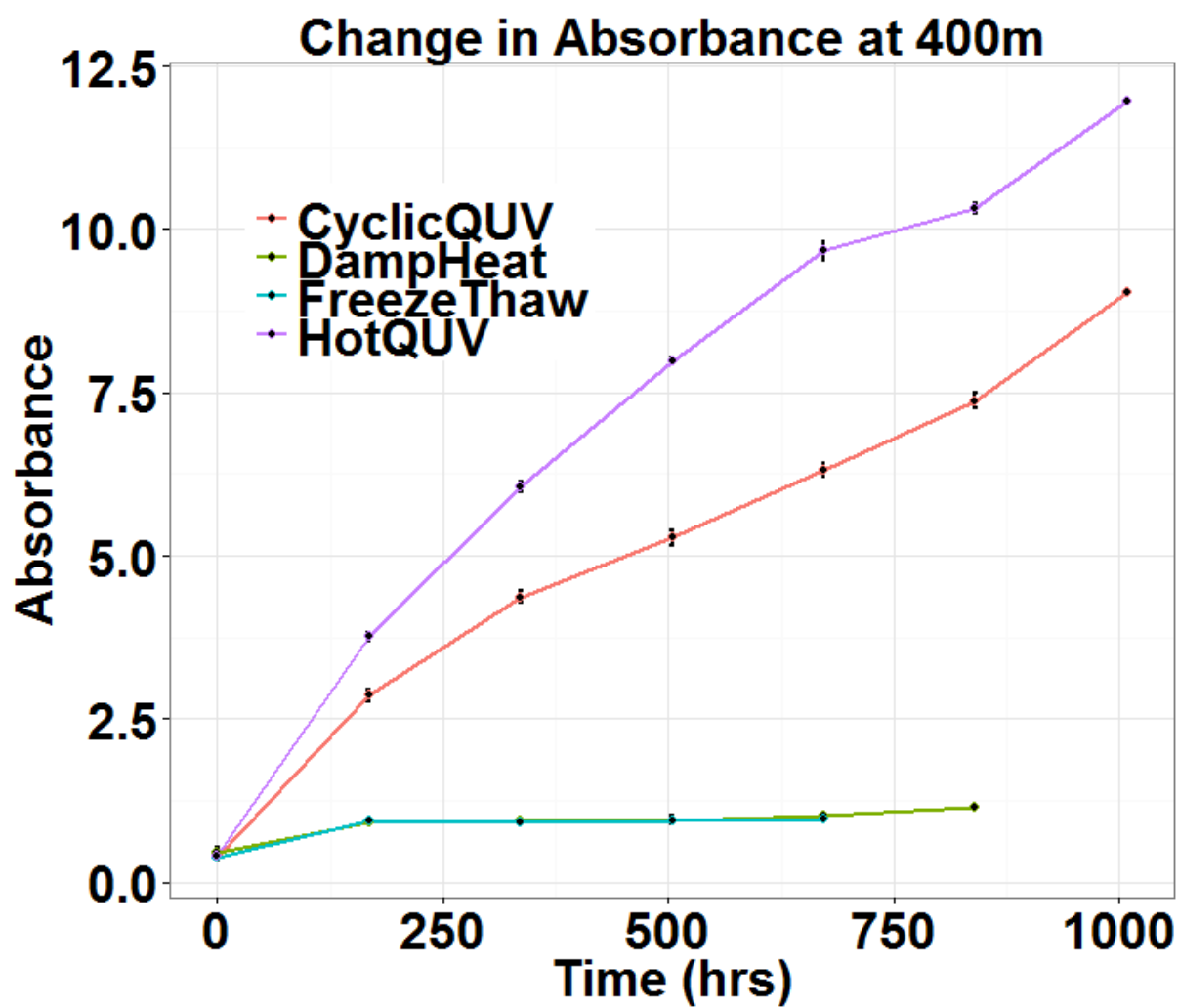
Figure 20: Figure
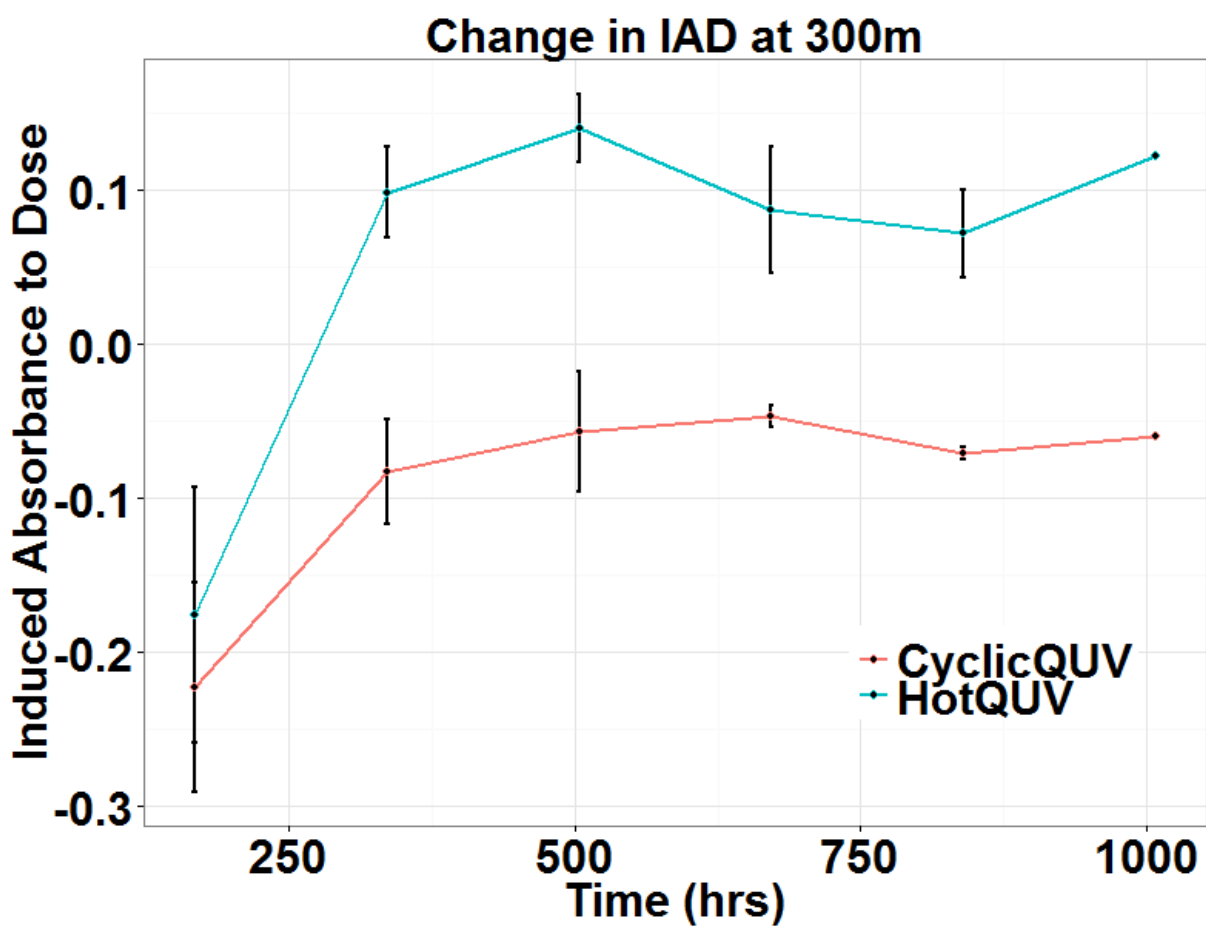
Figure 21: Figure
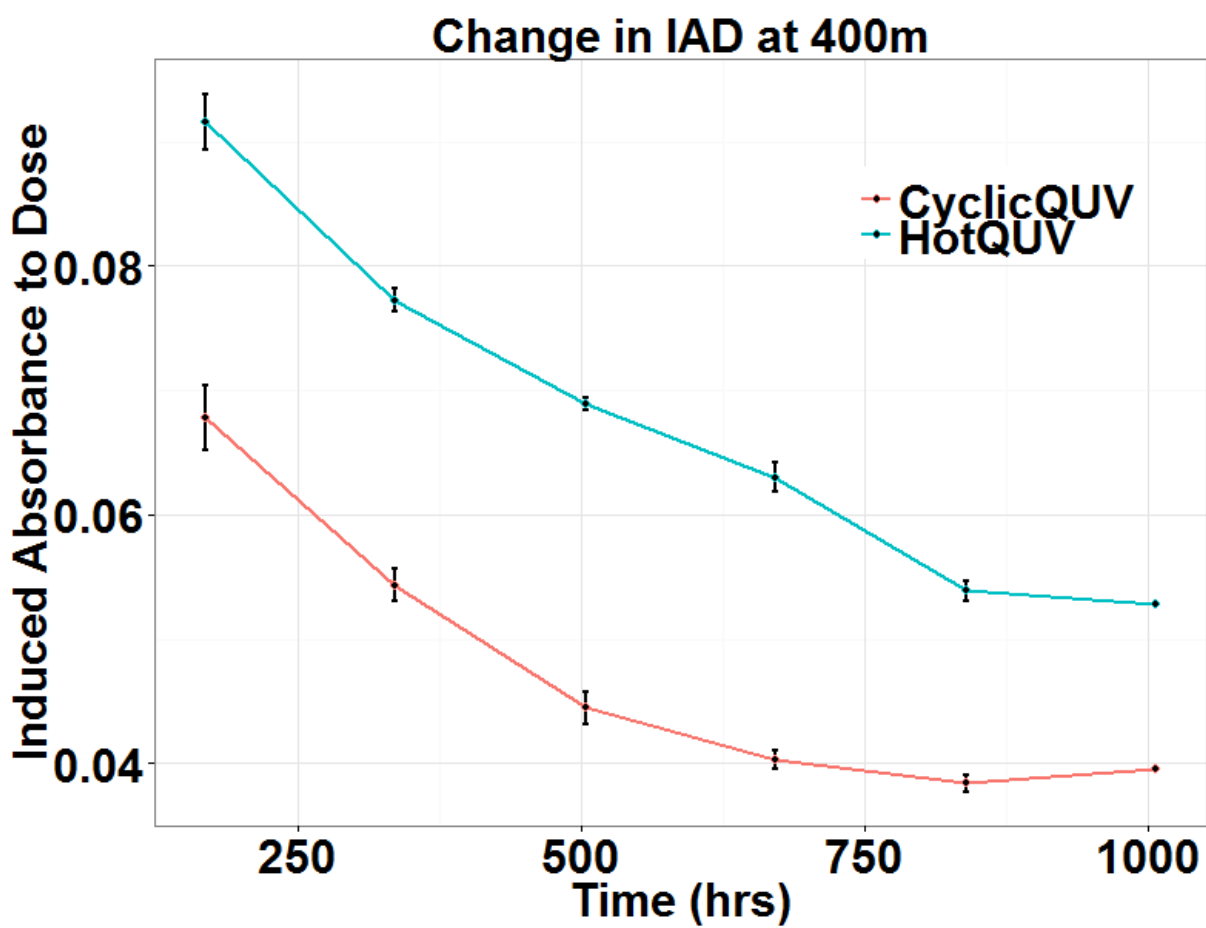
Figure 22: Figure
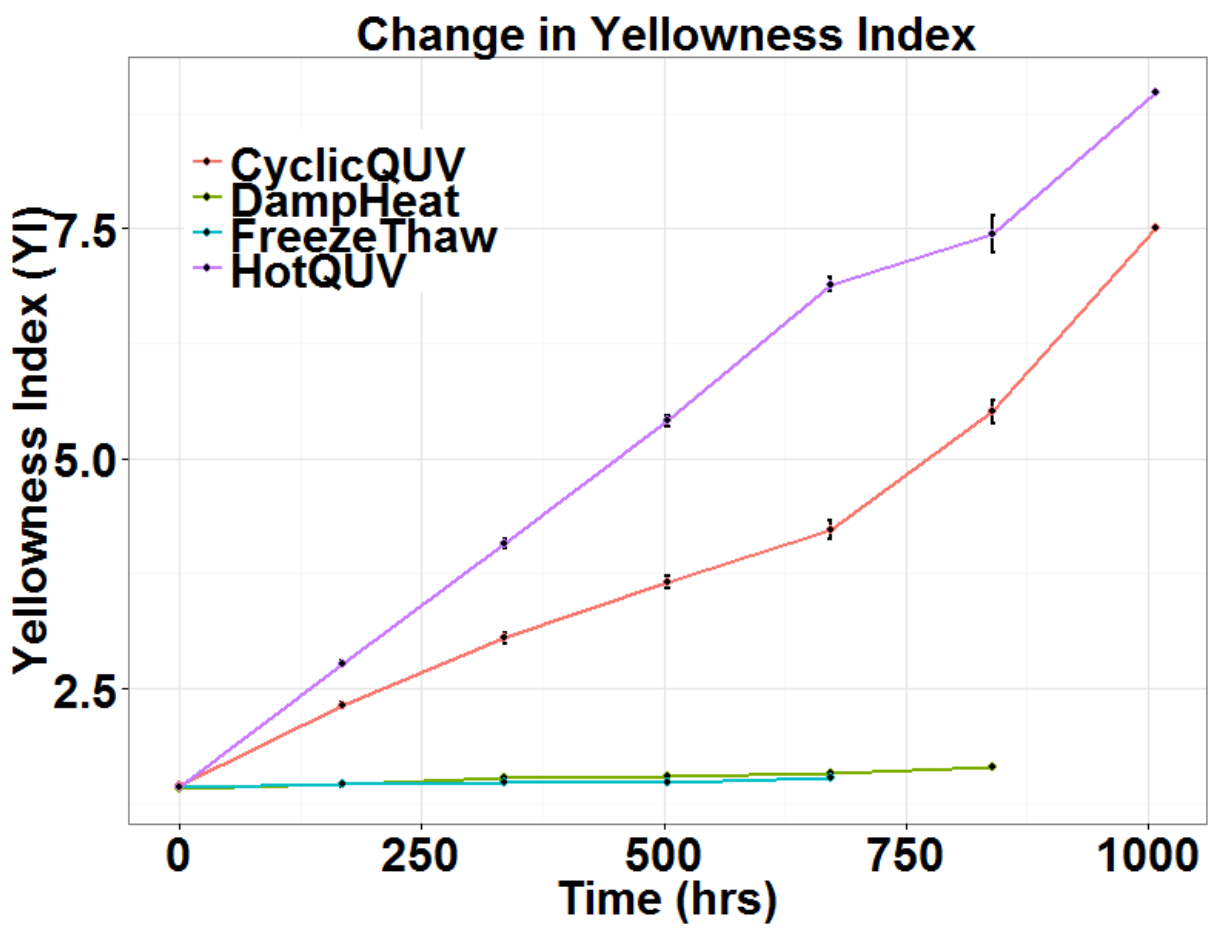
Figure 23: Figure
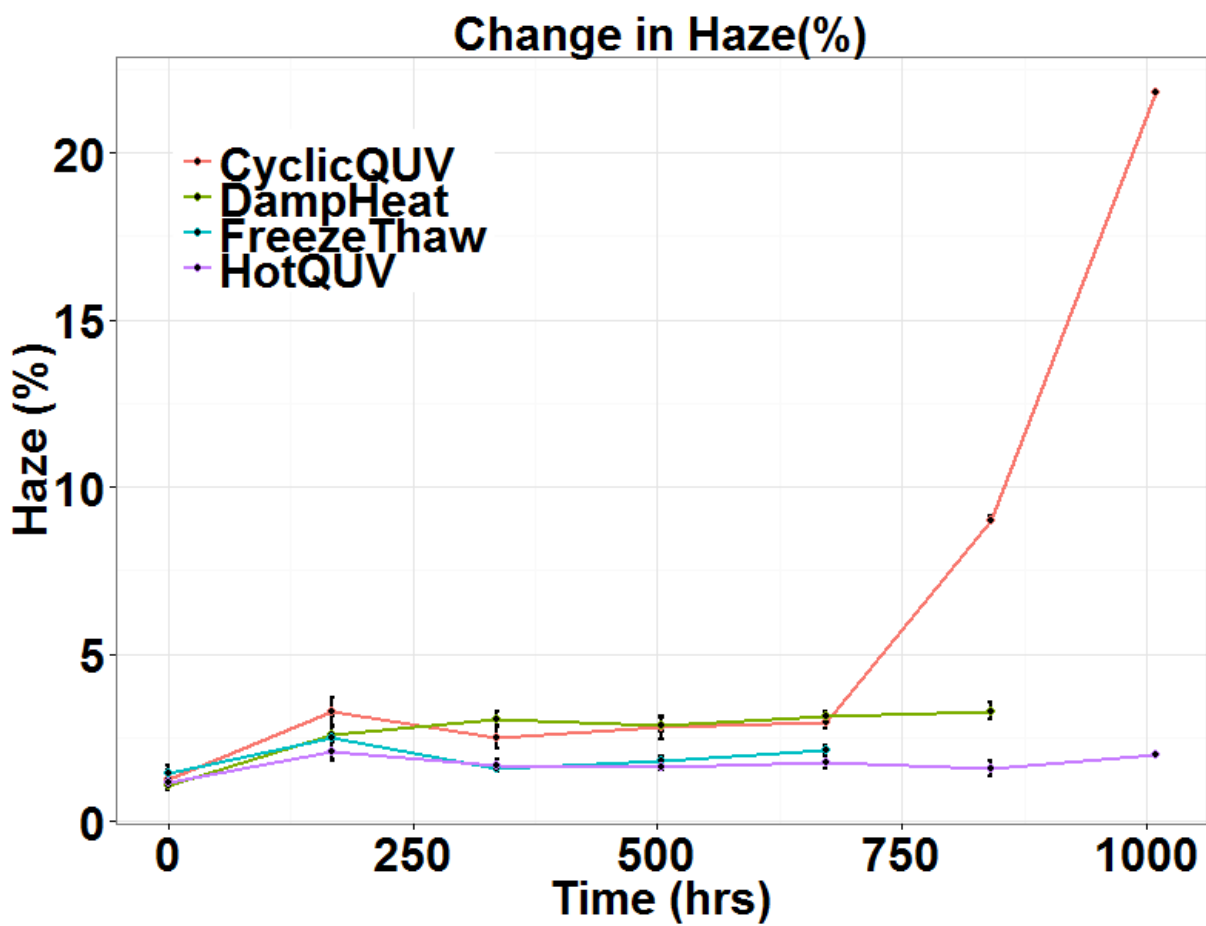
Figure 24: Figure

5.1.3.16 Comments

- Light induced yellowing in light exposures (con't UVA and cyclic UVA)
- Moisture induced hazing (cyclic UVA and damp Heat)
- It's more detrimental when light and moisture are coupled
- Freeze thaw is the less damaging
- Change point observed in the UV stabilized PET due to stabilizer consumption in light exposures.

5.1.3.17 Concluding Remarks

- R is a powerful tool!!!

5.1.3.18 Update on PetDegr Materials

- Six candidate materials and seven exposures

Exposure	Condition	Status
Outdoor 1X	1X conc. on dual axis trackers	Ready
Outdoor 4X	4X conc. on dual axis trackers	Ready
Continuous UVA	Constant exposure of UVA light at 1.55 W/m^2 at 340nm at 70°C	Ready
ASTM G154-4	Cyclic exposure of UVA light at 1.55 W/m^2 at 340nm at 70°C for 8 hours and condensing humidity at 50°C in the dark for 4 hours	Ready
Modified Damp Heat - IEC 61215	Constant exposure x°C / 85% RH exposure	Temperature TBD
Modified Humidity Freeze - IEC 61215	Cyclic exposure of y°C / 85% RH and -c°C / 0%RH	Temperature TBD
Multi-Factor	Full spec. light, heat, and humidity	Temperature and humidity TBD

5.1.3.18.1 Update on PetDegr Materials

- Baselining is ongoing

Evaluation	Instrument	Technique	Progress
UV-Vis-NIR Optical spec.	Cary 6000i with DRA (200-1800nm)	Center mount absorbance	DOne
UV-Vis-NIR Optical spec.	Filmetrics PartsUV (200-1100nm)	Direct T% and specular R%	Done
Color Measurement	Hunterlabs UltraScanPro (350-1050nm)	CIE $L^*a^*b^*$ Color - YI and Haze	Done
Gloss Measurement	BKY Gardner Micro-TRI-Gloss	20-60-85° Gloss	Done
Scattering BRDF and BSDF	ScatterMaster	Transmissive and Reflective Scattering	Done
Fluorescence Spec.	Cary Eclipse Fluorimeter	Fluorescence Spectra	Developing method
Nanoindentation	Agilent Nanoindenter G200	Elastic modulus and hardness	Developing method
Infrared Spec.	Agilent Cary 630 FTIR	Diamond ATR-IR Spectra	Developing method |