

# Predictive models for Service Life of Architectural Waterborne Coatings under Multi-factor Accelerated Weathering Exposures.

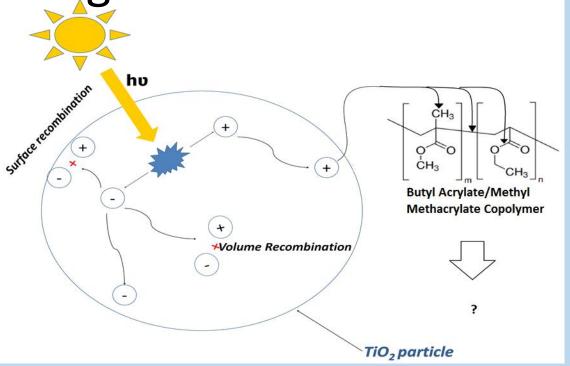


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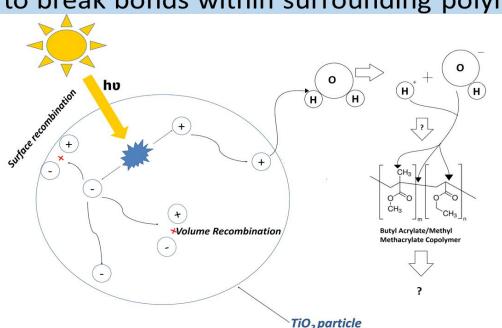
## Introduction

- -exterior waterborne acrylic coating systems concern the durability significantly.
- -The goal of this study is to investigate the effect of TiO<sub>2</sub> pigments on the photodegradation of polyacrylate system and build up a structural equation modeling for lifetime prediction
- -use FTIR to tracks the functional group changes as a material degrades.
- -build a R package to analyze the data from different FTIR data -use semi-gSEM to predict the degradation.

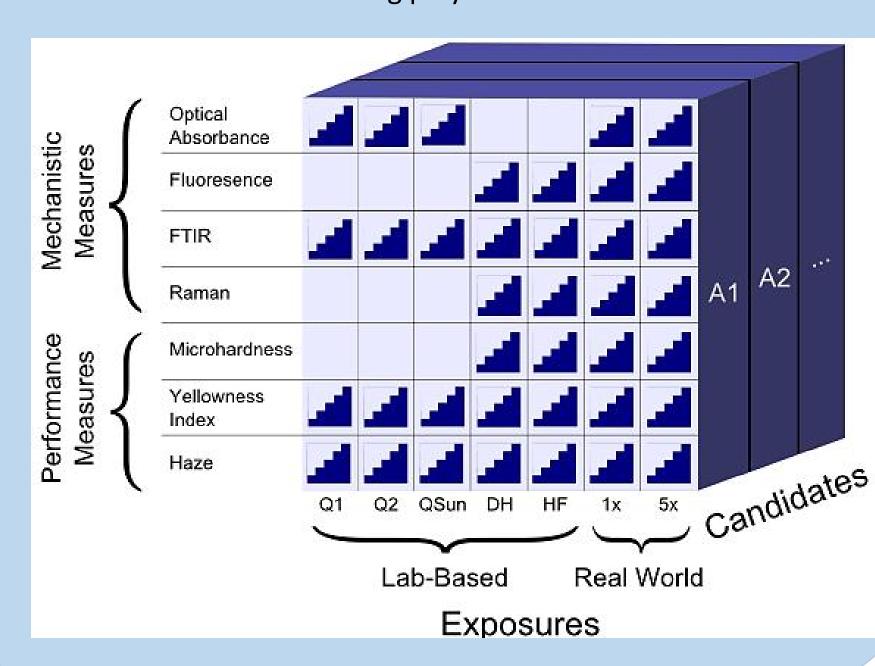
## Degradation mechanisms



**Mechanism 1**: UV light strikes a  $TiO_2$  particle, exciting its valence electrons, giving them a chance to escape the band gap of  $TiO_2$ . These escaped electrons will act as free radicals to break bonds within surrounding polymer.



Mechanism 2: Water is present, and excited electrons ionize the water into very reactive *H H* +and *O O* -ions, which quickly break down surrounding polymer.



## Results and Discussion

#### baseline correction:

- remove the background noise of impurity in the air. Normalization:
- bring the loudest peaks of the signal up to the highest level **Deconvolution:**
- decompose the peaks that overlap with each other, extract information about the "hidden peak".

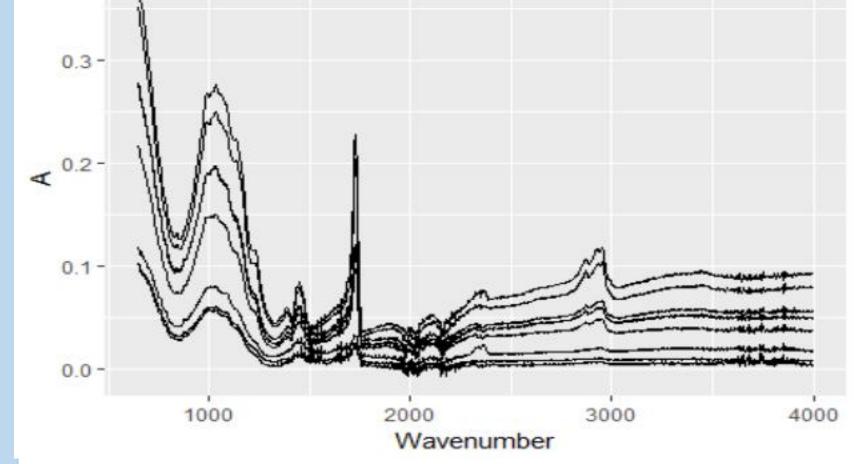
#### PCA:

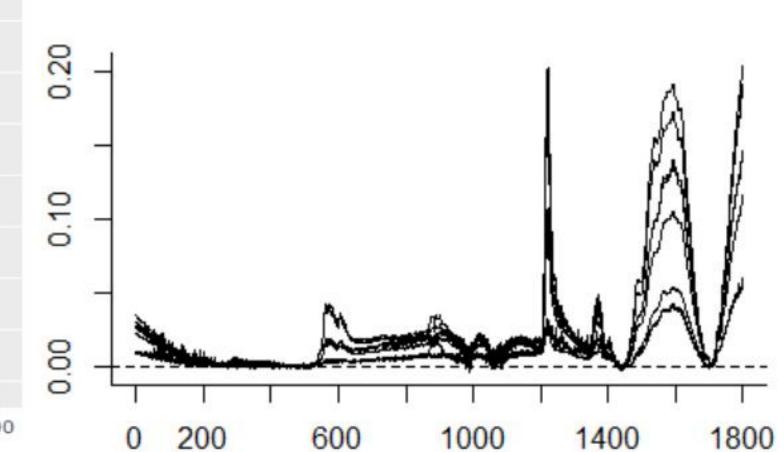
- reduce the multi-dimensionality of the FTIR data
- into its most dominant components or scores
- maintaining the relevant variation between the data points.

## To predict the degradation mechanism with quantitative FTIR data

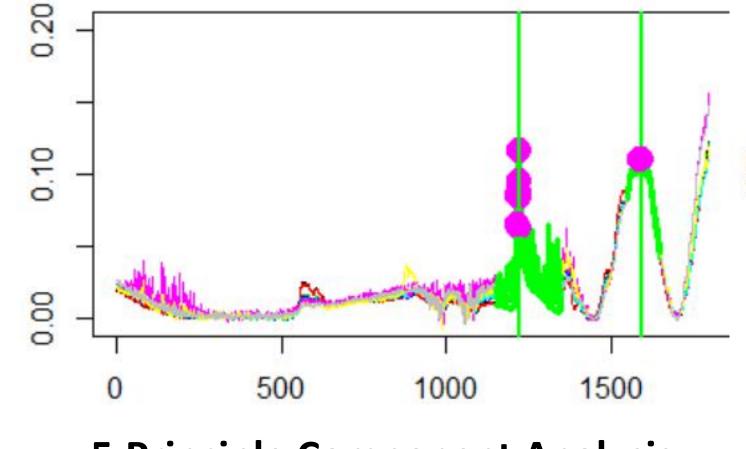
-mixed/fixed effects models and netSEM models are built to find the relationship between measured responses and length of exposure time under different exposure conditions.

## 1.Original data with different baseline level 2.Baseline correction

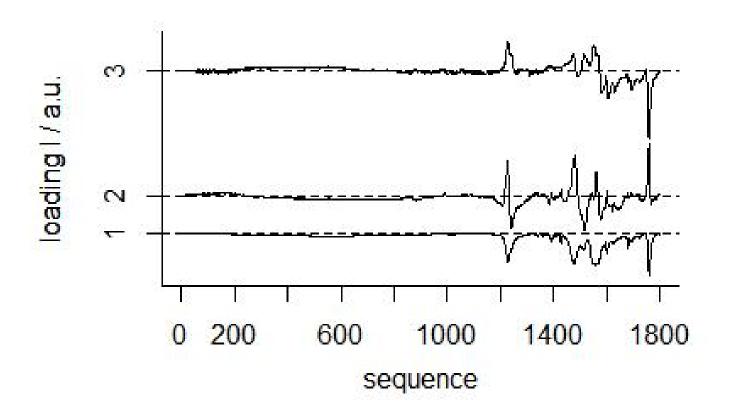




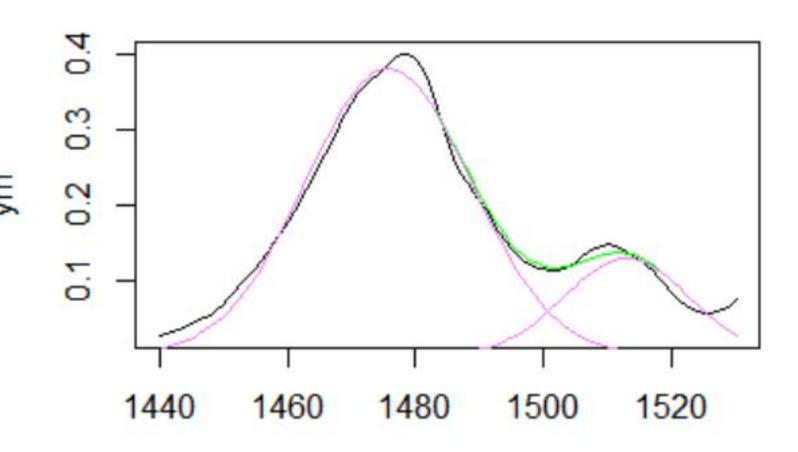
## 3. Normalization & peak ratio calculation



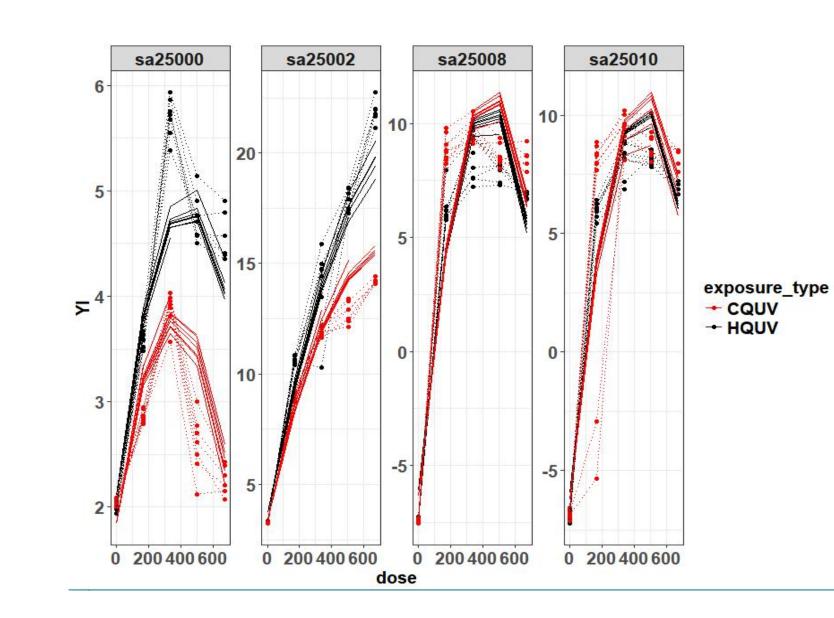
#### **5.Principle Component Analysis**



## 4.Deconvolution



#### 6. Modeling methodology



## Define peaks(literature review)

Baseline correction

Normalization

Deconvolution

PCA Analysis

ANOVA testing

### Peak Ratio, FWHM, Integral

Mixed-Fixed Effect

NetSem Model

## Conclusion

- 1.FTIR data shows the degradation tendency of carbonyl group along with exposure
- 2. after baseline correction/ normalization/deconvolution, PCA analysis, the curves on the FTIR data are smooth, on the same baseline and easy to be quantitative.
- 3. Calculate peak ratio/full width at half maximum/integral of a Gaussian function in R. Those responses are very important to present the degradation tendency.
- 4. Peak ratio of carbonyl group and C-O group, as mechanism in semi-gSEM modeling, shows relative strong relationship with stress, which is time of illumination

## Future Work

1.Use other general model to find correlation between predictors and response

## References

- 1.Allen, N. S., et al. "The durability of water-borne acrylic coatings." Polymer degradation and stability 47.1 (1995): 117-127.
- 2. Bruckman, Laura S., et al. "Statistical and domain analytics applied to PV module lifetime and degradation science." Access, IEEE 1 (2013): 384-403.
- 3. Abdulkerim Gok ,Laura S. Bruckman.,et al. "Predictive models of poly(ethylene-terephthalate) film degradation under multi-factor accelerated weathering exposures."

## Acknowledge

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- 2. SDLE