



# In-Situ Raman Spectroscopy Component Identification for Machine Learning Based Decomposition Analysis



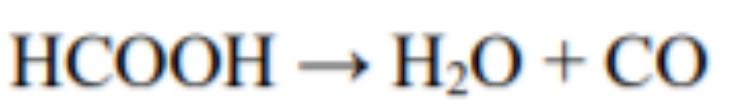
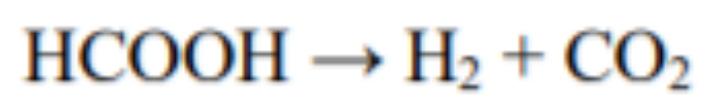
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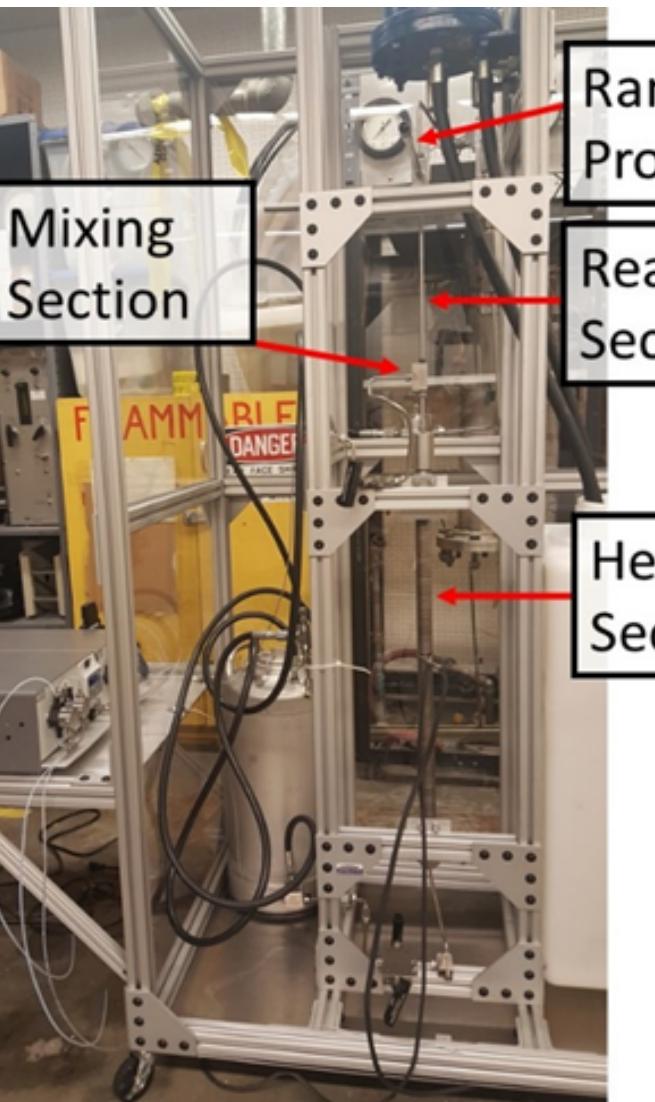
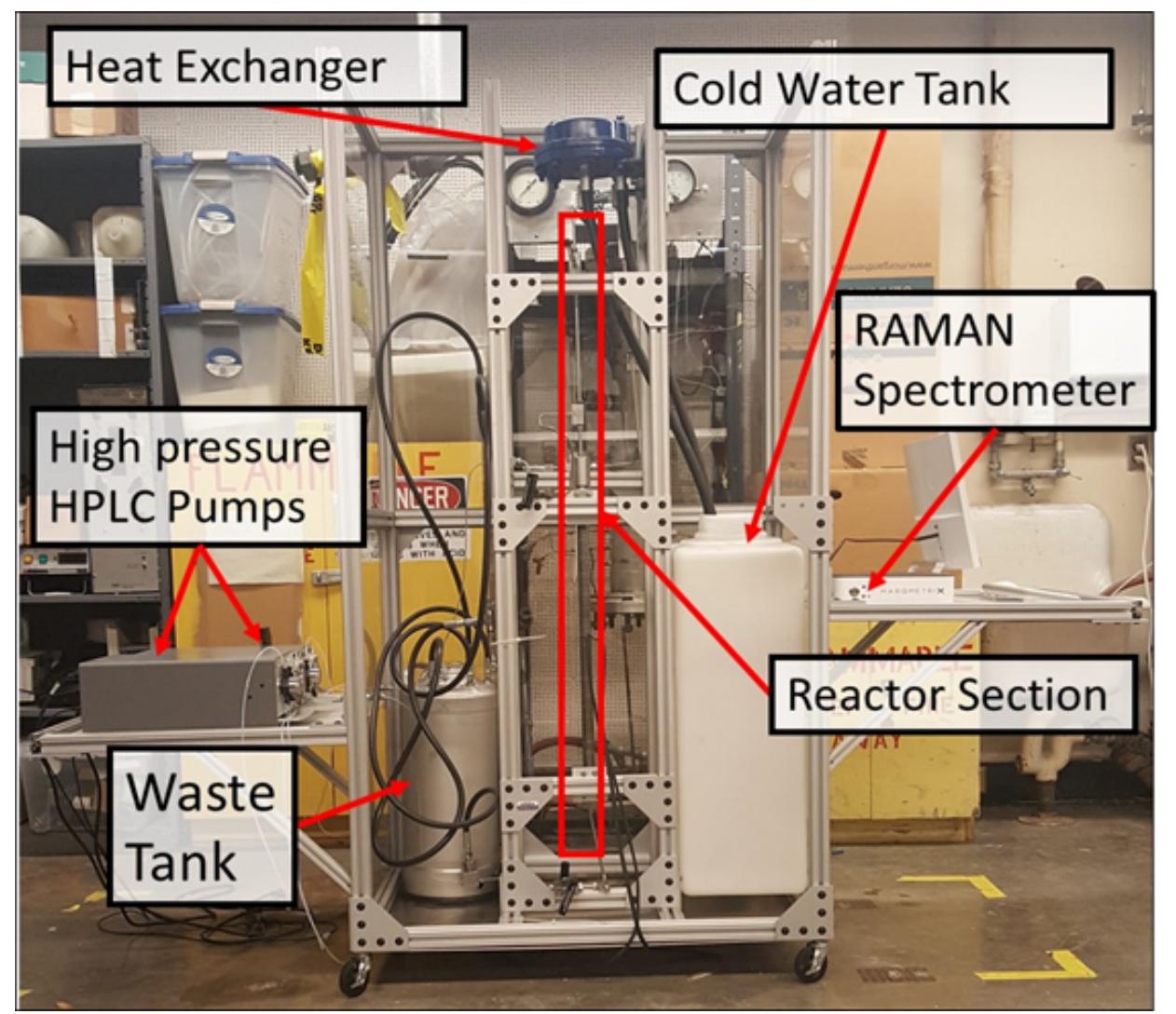


## Introduction

- Using data from a custom built supercritical gasification reactor on campus to analyze formic acid Raman spectra.
- Decomposition of formic acid constitutes the combination of two pathways:



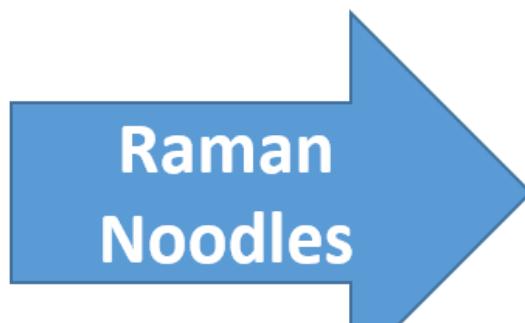
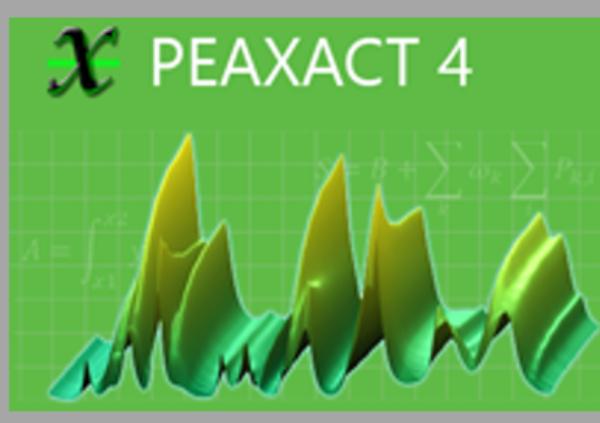
### Photographs of UW Gasification Reactor with In-Situ Raman Probe



### Motivation

#### Prior Analysis Method

- Commercial Software suite with yearly license cost of ~ \$3,000
- Not Open Source → Research backbone can be out of date
- Very tedious manual processes



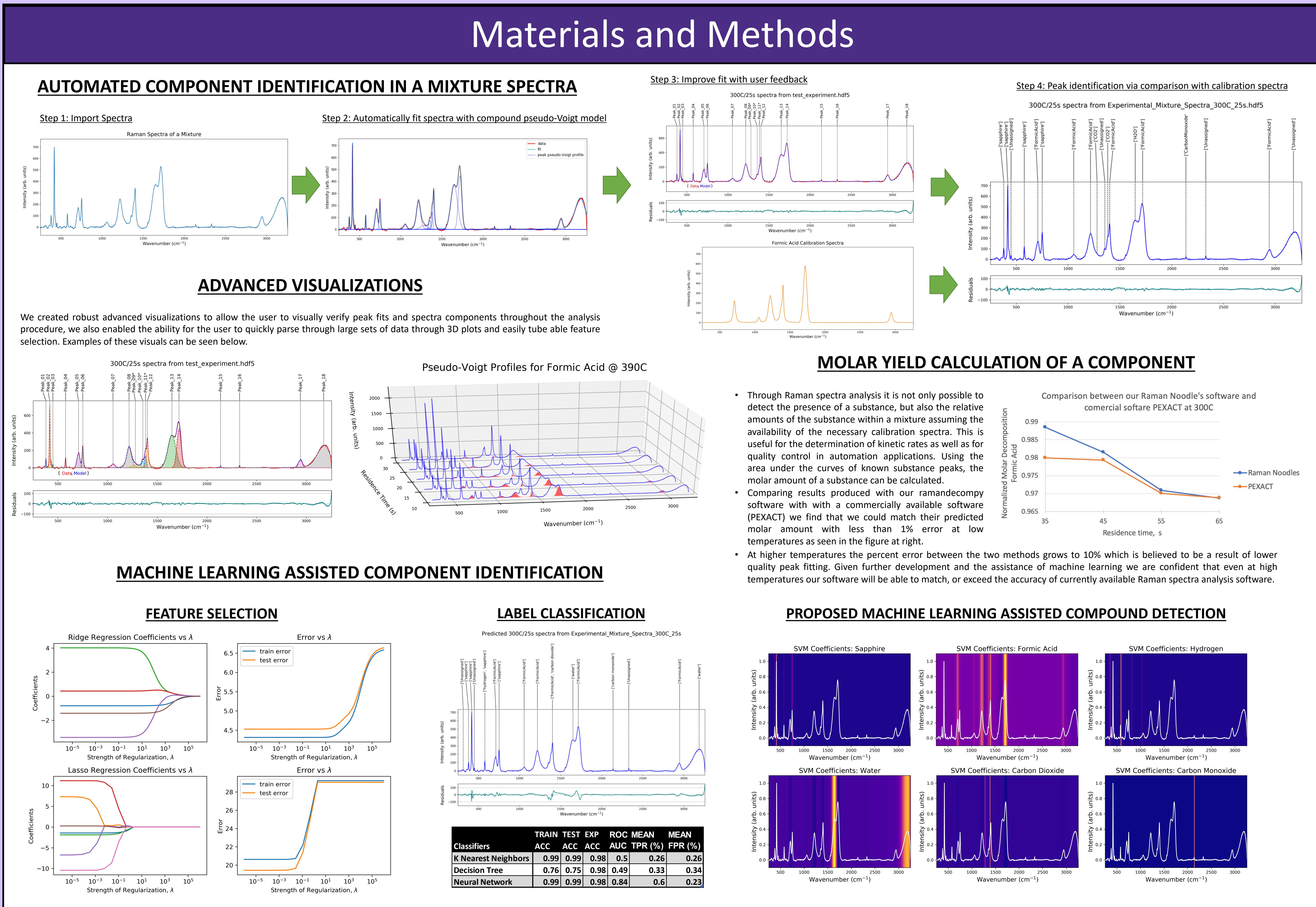
#### New Method!

- Free
- Open Source + Customizable → Research backbone easily updated by anyone
- Automated processes



## Goals

- Data Mining and Baseline Subtraction
  - Importing open source data sets, create a library of spectra, uniformly format data for analysis
- Data Visualization
  - Outputting plots of baseline subtraction and peak identification
- Machine Learning
  - Prepare least squares regression model for calculating kinetic rate decomposition at different resonance times and temperatures



## Conclusions and Future Work

In conclusion, our team successfully developed a complete, open-source solution for automatically fitting and labeling Raman spectroscopy data, organizing experimental and calibration spectra data, calculating decomposition values for chemical species, and easily producing useful plots of the results.

Future work: We hope that further development of our augmented dataset machine learning approach will allow for improved performance of our software and bring us even closer to a fully automated process

## Acknowledgements

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- Data sets from publicly available from Mendeley Data, "Raman Spectra of Formic Acid Gasification Products in Subcritical and Supercritical Water"
- Only open source packages were used in this work, documentation of all packages used can be found at our GitHub at:
  - <https://github.com/raman-noodles/ramandecompy>