Data Analysis of Biomass Isotopes Release During Thermal Conversion of Biomass

Member: Dingning Liu, Min Kim, Yutian Yang, Ziqin Wang
Client: Dr. Peter Thy, project scientist, Department of Earth and Planetary Sciences

Introduction

- Biomass is plant-based material used as fuel to produce heat or electricity.
  - Processed into solid, liquid, or gaseous fuels
  - Wood, wood residues, energy crops, agricultural residues, and waste from industry, farms, and households

- The utilization of renewable biomass for energy generation has distinct strategic, economic, and environmental advantages

Scientific Background

- Biomass is composed of wet biomass, dry matter (moisture), volatile solids (carbon, hydrogen, oxygen, nitrogen, etc.) , volatile matter (char: fixed carbon), ash (metals, minerals, etc. (silicon, aluminum, iron), and structural components (pectin, cellulose, lignin, etc).

- Biomass conversion
  - Thermal treatment of biomass materials enables the release and migration of elements.
    - Temperature varies by heating value and moisture content of fuel
    - Main elements released: carbon, hydrogen, oxygen

- Chemical reactions during thermal treatment
  - Organic decomposition
  - Char, carbonate, oxide formation and breakdown

Experiment of thermal conversion of biomass

- Project “Direct Monitoring of Elemental Losses from Thermal Conversion of Biomass,”
  - Connecting Differential Thermal Analyzer (DTA) to Inductively Coupled Plasma Mass Spectrometry (ICPMS)
  - DTA operated using a 200ml/min carrier gas flow of argon and constant heating ramps between 5 and 50°C
  - In each experiment, 10 to 15mg of biomass powder is heated continuously from ambient temperature often to 1300°C.
  - Connection of DTA to ICPMS allows detection of the temperature release of many metallic trace elements relative to the breakdown of typical biomass molecules, such as cellulose, hemicellulose or lignin detected by the release of carbon.

Project outcome and Scientific Goal

- Investigate predictability of the release of toxic metals from biomass and waste thermal conversion or treatment facilities, including improved understanding of feedstock pretreatment in attempting to control composition and volatile release.
- Identify the fundamental patterns in dataset obtained from experiment that are related to chemical reactions such as organic decomposition and oxide formation and breakdown as a function of increasing temperature.
- Investigate how metal release are related to different chemical reactions during the combustion and heating process of organic fuels.
- Data analysis project goal:
    - find the relationship between the release of isotopes and temperature and possible effect of other factors such as total mass of individual elements and their kinetic behavior.

Data Collection

Two sources: DTA and ICPMS.

The two datasets are synchronized and down-sampled.

Down-sampled data: 870 observations.

Variables:

- Time (s)
- Setpoint Temperature(C)
- Sample Temperature (C)
- Sample Weight (mg)
- Residual Mass Fraction
- Heat Flow (J/s)
- Released count of 55 isotopes.

Limitation

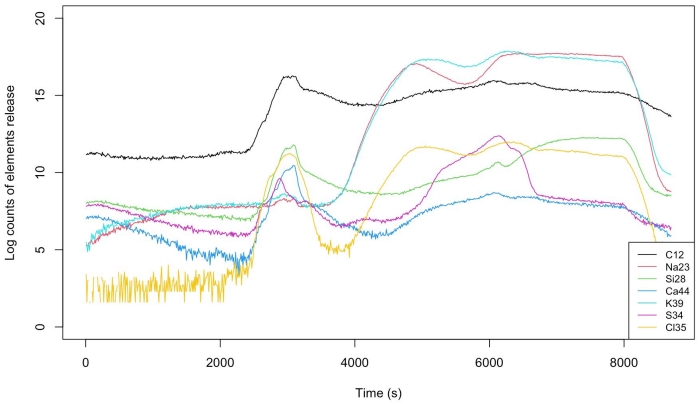
- Sample size

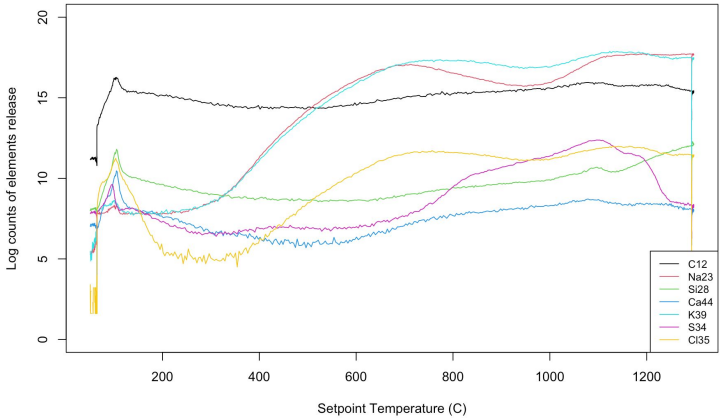
  Collecting more samples (5-10 combustion process) would increase robustness of statistical results.

- Correlation between time and temperature.

  Adjusting the heating rate so that temperature can be unchanged for a period of time would make our results more reliable.

Exploratory Data Analysis





Previous Work

Machine learning techniques have been widely used in modeling of combustion, gasification, and pyrolysis processes.

- Ji and Deng proposed a chemical reaction neural network (CRNN) to interpret reaction pathways and quantify kinetic parameters simultaneously from the weight of the neural network.
- Kardani et al. compared Extreme Gradient Boosting method (XGBoost), Multilayer Perceptron Artificial Neural Network (MLPANN) and Support Vector Machine (SVM) in predicting the conversion of any feedstock based on the composition and operating conditions.
- Aghaaminiha et al. showed that machine learning models are appropriate for interpolating and extrapolating the kinetics of the HTC process but deviated from experimental data under certain conditions.

Modeling: Random Forest

- Our goal: To identify fundamental patterns in the dataset related to chemical reactions.
- Random forest is a decision tree-based ensemble learning method that performs both classification and regression tasks.
- Random forest can achieve this goal by clustering isotopes into different groups based on its clustering algorithm.
- After clustering isotopes, we can look into each clustered group of isotopes that share similar properties.
- For example:
    - Time <= 2000s
    - Total mass of the individual element <= 20mg
    - Isotopes whose release count >= 10000

Modeling: Random Forest

- Step 1: using random forest methods for classification. This is intended for calculating the dissimilarity matrix (guideline metrics that include the independent variables like time, temperature, total mass, etc.)
- Step 2: implementing Random Forest on unsupervised learning, meaning that the model will assign clusters to the observations according to the dissimilarity matrix without being prespecified.

Furthermore, we could keep utilizing the potential relevant predictors to improve the results.

Modeling: Result

- Figure 1 shows that the isotopes are being clustered into four groups.
- However, there are not enough samples, we can observe a large amount of variations in Figure 2, in which case we are not able to draw robust statistical conclusions.
- Potential method:
  - calculate the weighted average of the clusters assigned for each isotope
  - compare the weighted average clusters
  - we cannot assume the conclusion is statistically significant.

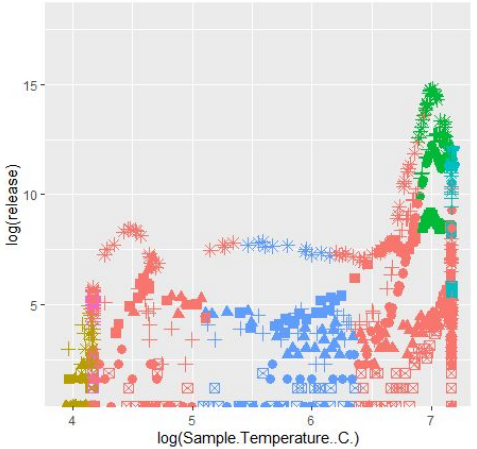


Figure 1

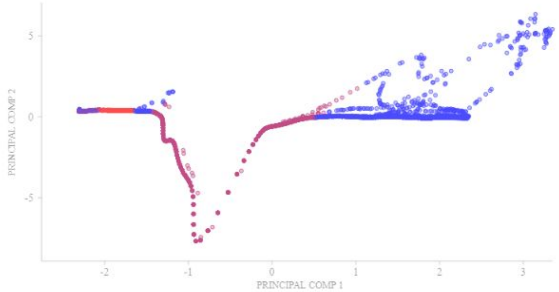
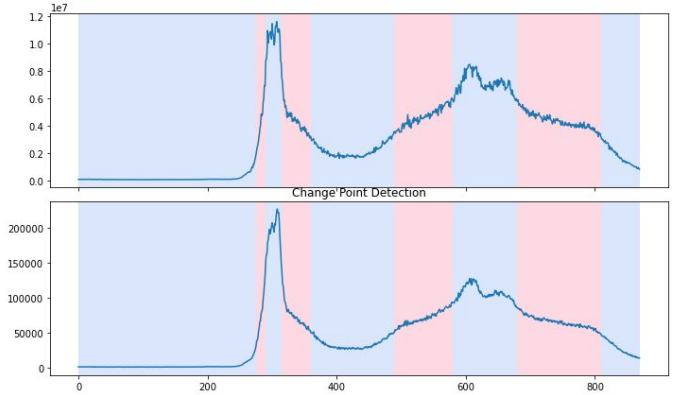


Figure 2

Ruptures Package in Python

- Rupture is used for change point detection of Time Series datasets
- Example: Change point detection of C12 and C13
    - C12 and C13 have a very similar distribution of release and thus they have the same change points, which suggests that C12 and C13 are released together during the combustion, so we should group C12 and C13 together.
- We can compare the isotopes pairwisely to conclude the pattern of isotopes released together under different time (or temperatures)
- Drawback:
    - Only taking consideration of time and release but ignoring other useful factors like total mass and kinetic behavior.
    - Does not take into account the amount of release.



Change points detection of C12 and C13

Conclusion and Discussion

1. We proposed clustering and change point detection to identify the fundamental release pattern of isotopes during combustion of biomass, and we conclude there are 4 groups of isotopes with similar properties, also change point detection approach help us compare the change point of the release of each isotope during the combustion pairwisely.
2. The problem is that both methods provide us with some general ideas, but the result is not solid enough because of the limitations brought by the sample sizes, if in the future study we could collect a larger sample with more relevant factors, then it is likely to provide a more accurate clustering results.
3. Additional clustering methods could help us investigate how isotopes are released under different chemical reactions throughout the combustion and heating process.

Acknowledgement and contribution

We take this opportunity to express my sincere gratitude to Prof. Bala, Dr. Thy, Dr Jenkins, Ben, and Tianke for their valuable guidance and kind help throughout.

- Dingning: Scheduled and held Zoom meetings, write-up proposal, initial statistical analysis (transformed additive model). Introduction, previous work, data collection, limitation,EDA, and conclusion of the report.
- Min Kim: Document organization, communication with teaching team and client, Write-up proposal. Introduction, scientific challenges and goals, and data collection of the report.
- Yutian: Write-up proposal, statistical background, EDA, Random Forest modeling, Ruptures, results, limitation, and conclusion of the report.
- Ziqin: Initial statistical analysis (linear and Poisson) and draft conclusion of project.

Thank you!