Project Proposal

A Pinch of This, a Dash of That: Optimization of Food Waste Feedstock for Anaerobic Digestion

1. Proposed Idea

Microbial anaerobic digestion (AD) is the key mechanism to convert organic wastes into energy in the form of biogas (CH_4). Traditionally, the organic waste being utilized for biogas production is composite waste water and activated sludge from municipalities, however, food waste is another large organic waste stream that could serve as a viable feedstock though the composition of food waste is highly variable and complex, making it difficult to utilize consistently. However, as the compositional data of common food wastes continues to increase it is becoming more feasible to model and predict biogas production when the food waste composition is known. In this project we will utilize the generic structured anaerobic digestion model (ADM1) [7,8] to simulate the biogas production of common food waste feedstocks individually and as combinations to assess the chemical composition for optimum biogas production over a standard period. We will specifically investigate the ratios and quantities of the principal chemical components: carbohydrates, lipids (aka fats), and proteins, and how each component's relationship impacts the overall production. <u>Our specific research questions are as follows:</u>

- What is the correlation between the principal chemical components of the food and biogas production?
- Are there consistent factors (i.e. ratios of the principal chemical components) that amount to high biogas production?
- What combinations of food waste feedstock ingredients achieve the highest production of biogas and how does this compare to individual feedstock ingredients?

<u>The dataset that will be utilized has the following characteristics:</u>

- **Source:** The primary dataset will be the chemical compositional profile of common food waste items which will be taken from publicly available published literature such as Slopiecka et al 2022 [1].
- **Type:** The original data will be stored as a CSV, structured as a table of rows and columns where rows will be the food waste item and the columns will be the chemical component e.g. carbohydrates, proteins, lipids, etc.
- **Size:** The most complete dataset identified is the Slopiecka et al 2022 dataset. This contains 88 food waste items, each with a name and chemical profile consisting of 12 chemical characteristics. This makes the original dataset an 88 x 13 matrix. Our initial investigation will focus only on the principal chemical components (carbohydrates, lipids, and proteins), which narrows this down to an 88 x 4 data frame. We will use ADM1 to generate an estimate of biogas production potential for

each food item, and these estimates will comprise another data column. For consistency, we will also assign a unique numerical ID to each food item, bringing the total to an 88 x 6 data frame. When considering combinations of food waste items, each pairwise combination will be put into a new row with its own features. With 3,828 pairwise combinations and 88 original items, the result is a 3,916 x 6 data frame.

The team has the following members:

Robert M Jones: conceptualization, data curation, methodology, visualization, formal analysis, writing (drafting, reviewing, editing): Robert is trained as a microbiologist and is currently pursuing a PhD studying anaerobic digestion of complex substrates. He has experience working with the ADM1 model, bioinformatics, and data visualization

Nate Borland: methodology, software, visualization, formal analysis, writing (drafting, reviewing, editing) : Nate is an experienced software developer pursuing a Master's in Complex Systems & Data Science. Nate has experience with software development, data analysis and visualization, and version control tools.

To stay on track of the key project assignments we have the following task timeline

Task	W1	SB	W2	W3	W4	W5	W6	W7	W8	W9
Data acquisition and cleaning										
Model code editing, formatting, and loop initialization										
Mono-feed modelling and output aggregation										
Mono-feed data analysis										
Project Check in #1 (24 March)										
Paired-feed code editing, formatting, and testing										
Paired-feed modelling and output aggregation										
Project Check in #2 (7 April)										
Paired-feed data analysis										
Report Drafting										
Project Check in #3 (21 April)										
Report editing and finalization										
Report complete										

Communication and Data Management:

- Communication - In-person and on Microsoft Teams when remote
- Version Control - Code and data files will be managed through a GitHub repo

- Citation Management - The final report will be assembled in Overleaf, with a .bib file used to track citations
- Naming Conventions - The data files will be named food_waste_data_raw.csv for the unaltered data, food_waste_data_trimmed.csv for the version with only the principal chemical components, food_waste_data_biogas.csv for the version with biogas production added, and food_waste_data_combinations.csv for the version with combinations of food items and their biogas productivity. If necessary, a version number (i.e. _v1) will be appended to the end of the file names.
- Data Management - Data files will be stored locally and managed with git

Ethical Considerations:

The datasets in question are publicly available and represent aggregate data of the chemical compositions of food waste [1]. As such, they do not contain any information pertaining to specific individuals or groups of people and do not contain any PII or sensitive information. What will be the most important ethical considerations for us will be the consistent and accurate crediting of the data sources and their original authors. We will do so by establishing consistently and frequently that the data in question was not produced by us and provide permanent means of accessing the original data (DOI) and consistently citing the authors.

2. Preliminary Literature Review

As global populations continue to increase, both waste management and energy production are becoming challenging issues [2]. The conversion of food waste into biogas is a sustainable mechanism that can alleviate both issues at once by reducing the volume of food waste entering the uncirculated waste stream (landfill) and providing a source of renewable energy in the form of biogas [2]. While currently there are relatively few waste facilities specifically devoted to producing biogas from food waste they are capable of producing energy on the order of tens of thousands of kilowatts [3]. While advancements have been made there are still many challenges facing the production of biogas through anaerobic digestion primarily due to the uncontrolled variability in the chemical composition of food waste streams which are not conducive to consistent biogas production, may cause inhibitory reactions, or lack the nutrition necessary for complete digestion [4]. For the production of biogas the primary chemical constituents are carbohydrates, lipids, and proteins [5] and the relative amounts of these are integral in biogas production [6]. For example, while high carbohydrates provide ample material for biogas production, the presence of high proteins can result in ammonium production that inhibits the overall production rates [6]. The anaerobic digestion process is highly complex with an array of commensal, dependent, independent, and inhibitory reactions occurring across time that influence overall biogas production making the predictions of biogas output challenging. However, generic models such as the Anaerobic Digestion Model No.1 (ADM1) have been successfully utilized to provide base predictions of biogas output given the chemical composition of the feed with high accuracy [7,8]. The ADM1 model has been used to model food wastes as well as a variety of other nontraditional waste streams (agricultural wastes, industrial wastes, specific process wastes) [9-12] but less research has been done on understanding and modelling the particular value of each food waste item as a mono-component or in aggregation [9]. As previous research has shown, the types of food in the digestible waste are highly determinant of the biogas production and each broad sector of food attributes specific qualities to the overall waste composition, ex: dairy products contribute large amounts of fats, while breads and produce introduce carbohydrates [9,13]. However while these general impacts of food categories are known, what is less studied that will be investigated in the proposed research is the biogas potential of individual food items which can be utilized to better understand how complex food waste streams will produce biogas when the items are in a realistic aggregate.

3. Project Suitability

Throughout this project the team will draw upon and actualize many of the fundamental methods, and practices that have been taught in this course. Fundamentals and practices such as data acquisition (acquiring data from the original source, tracking provenance, and performing appropriate attribution), data cleaning and manipulation (transforming the data to be appropriate to use in the downstream software and models), and methodologies such as using dimensionality reduction to create coordinate plots that can be used to visualize complex data. For example, to understand the relationship of the chemical characterization to biogas production we intend to create a 3-dimensional non-metric multidimensional scaling plot which will allow us to visualize clusters of similar food waste items and assess the commonalities of their relations. Additionally, a significant portion of the class covers the utility of models in data science and the keystone of this project is the anaerobic digestion model which will be the primary engine for data output. This model is a mathematical model that incorporates a series of first order rate equations for the multitude of components involved in anaerobic digestion and typifies the function of a model discussed in class i.e. to aid in predicting outcomes (biogas production) given known data (food waste chemical composition).

4. Research Significance

The amount of food waste in most developed countries is astronomical and results in a massive amount of landfill bulking and greenhouse gas production [15]. Apart from being wasteful and harmful to the environment, food waste also represents a substantial loss in resources as it has the potential to be recovered through biological mechanisms and converted to various energy providing forms e.g. biomethane and biohydrogen [2,4,15]. Anaerobic digestion is one of the most efficient mechanisms at recovering energetic resources from food waste and is increasingly considered as an alternative waste management strategy to aid in meeting sustainability goals [14]. However, characterizing and predicting the biogas output from food wastes is challenging due to the variable composition [1,13] and the changes in biogas potential that individual food items contribute to biogas production is not completely understood. In utilizing the ADM1 model and existing food waste characterization data to simulate biogas production for theoretical food waste streams, we can begin to better understand how real-world aggregate food waste will produce biogas. In studying the biogas production of mono and pairwise combinations of food items we will begin to elucidate the synergistic and inhibitory properties that each food item may contribute to a food waste stream which can better aid in the predictions of biogas production.

5. Personal Growth Goals

My current PhD research is understanding how complex terrestrial substrates will undergo anaerobic digestion through the products that I am interested in are medium chain fatty acids not necessarily biogas (although biogas is a key component). In the course of that research I will need to become familiar with the complexities of anaerobic digestion which is in part the impetus for pursuing this project. My goal is to become proficient in the application of the ADM1 model, to understand how the primary chemical components influence biogas production. I also have limited experience in MATLAB which is the software in which the model is run and my goal is to improve my skills in navigating and executing MATLAB code to the point where I can be confident in pushing and pulling data into MATLAB, modifying existing code, writing loops, as well as writing and executing MATLAB functions.

6. Technical Requirements

Software, tools, and code

- MATLAB
- RStudio (Base R)
- ADM1 Model (MATLAB execution, Weinrich et al 2021)
- Excel
- Jupyter Notebook (Python)

Programming languages, libraries, frameworks

- MATLAB (MATLAB code C/C++)
    - ADM1 model, combntns, simulink
- Python (matplotlib, pandas, seaborn)
- R (ggplot, tidyverse, vegan)

7. References

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