Analysis and Development of a Laboratory-Scale Anaerobic Biodigester

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Abstract

Anaerobic digestion has the potential to reduce the reliance of fossil fuels for tasks including electricity generation, cooking, and heating. This process involves converting solid waste into renewable biofuels. Due to its complexity, a large focus has been placed on studying the theory behind anaerobic digestion and developing predictive models to evaluate its efficacy on different time and length scales. In this paper, we describe the use of mathematical modeling to develop and validate a simple and robust kinetic model for the process of anaerobic digestion. This mathematical model builds off of existing models in the literature through simplified consideration of both the system's kinetics and thermodynamics. The results of our kinetic model are promising, yielding similar results to two sets of published data with R^2 values of 0.94-0.95. In addition, we discuss the development of a low-cost and versatile laboratory-scale process to evaluate anaerobic digestion. Combined with our robust mathematical model, our work demonstrates promise for the use of anaerobic digestion technology as an effective contributor to sustainable energy production and waste management.

Introduction

The use of anaerobic digestion processes to convert solid food and animal waste into renewable energy has tremendous potential to reduce fossil fuel consumption and improve climate change trajectories. Anaerobic digestion involves the use of anaerobic micro-organisms to convert solid wastes into renewable biofuel that largely consists of methane. Due to its high energy content (~39.4 MJ/cm^3),[1] methane (CH_4) can be repurposed for a variety of energy saving tasks including heating, cooking, and electric production[2]. The effective conversion of food waste into useful biofuels depends on a variety of conditional factors including feedstock composition (C:N ratio), organic loading rate, temperature, pH, bioavailability, and hydraulic retention time[3]. Controlling these factors and studying the process of anaerobic digestion via experimentation is very complex and often involves mathematical modeling to allow for the interpretation of obtained results. *To evaluate the feasibility of anaerobic digestion, we* *simultaneously designed a mathematical model and proposed development of a laboratory scale anaerobic biodigester.*

Due to the complex relationships between biological processes and chemical processing conditions, describing the efficiency of anaerobic digestion through theory is non-trivial. On a biological level, the process largely depends on a complex synergistic relationship of different anaerobic bacteria to process different reactive feedstocks. The organic matter feedstock used in anaerobic digestion is largely composed of complex species like proteins, fats, and soluble lipids and, therefore, must be biologically broken down into amino acid monomers, fatty acids, and simple sugars[3]. The resulting products of this chemical hydrolysis feed into subprocesses termed acidogenesis, acetogenesis, and methanogenesis. Additionally, there are a variety of chemical processing factors that affect the outcome of biogas production including the accumulation of ammonia and volatile fatty acids in addition to changes in pH[3]. All of these complex factors combine to result in the disconnect between anaerobic digestion process conditions with theoretical predictions.

The ability to predict the performance and output quality of an anaerobic digestion process is largely dependent on the development of tools to study the process on a laboratory scale. Additionally, to correlate the efficiency of a process on the laboratory scale with that of an industrial scale reactor, for instance, robust mathematical modeling tools must be utilized. While the efficiency of the process is largely dependent on the feedstock conditions, the scale of the process can have an effect on the thermodynamic[3] and mass transport[2,3] properties -- all factors that must be accounted for when designing an anaerobic digestion process. A variety of approaches have been used to predict the kinetics of anaerobic digestion. This includes the development of sophisticated models in ASPEN that take many different factors into consideration. Such ASPEN simulations rely on advanced fluid mechanics, thermodynamics, and mass transfer computation that are not readily accessible by a wide range of researchers. Additional approaches include the application of more simplistic kinetic models like describing the process as a first order reaction that is assumed to occur in one step. In this work, we describe the use of MATLAB in the development of a simplified yet robust kinetic model that takes a variety of assumptions into consideration to report simple and meaningful results from laboratory scale to industrial scale reactor setups. Additionally, we propose a simple design for a laboratory-scale anaerobic digester. Although not yet experimentally validated, our design is low-cost and easy to construct.

Methods

Lab-Scale Anaerobic Digester Design

To study anaerobic digestion on the laboratory scale, a small 3.784 L system was designed and constructed (Figure 1A). The design of the system maintains a small footprint but also allows for versatile data collection of parameters including temperature, pH, and pressure via different Ardunio based sensors. The system was largely constructed using a 3.784 glass fermentation system obtained from Home Brew Ohio (Figure 1B). Additionally, a smaller mason jar was utilized as a gas collection container. The two containers were connected via ¼” PTFE tubing. In order to allow for purging of the air from the anaerobic digester, the plastic lid was modified in order to contain two ports, one serving as a purge port and the other as a connection to the biogas collection container. The purge port was connected to a 2-foot-long piece of ¼” tubing that is connected to a valve to allow for actuation of the purge stream. The purge tubing can be connected to a source of nitrogen to remove all the air present in the container upon charging with substrate. The lids of the apparatus were also modified to allow for accommodation of the pH, temperature, and pressure sensors as described in the next section.

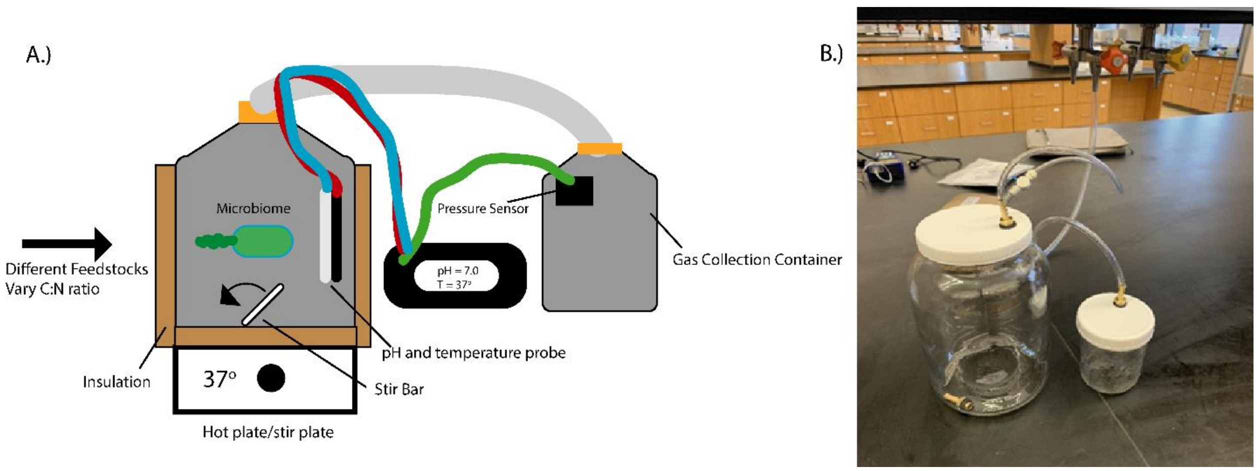

Figure 1: A.) Schematic *of the laboratory-scale anaerobic digestion process. The anaerobic digestion process occurs in a large (>3L) container that is connected to a smaller gas-collection container. The entire system is on top of a hot plate to maintain desired temperature conditions. Sensors to monitor, pressure, temperature, and pH are mounted inside of the container so that response conditions are observed.* B.) *Components of the pilot digester pre modification of the lids. This depicts the 3.784 L fermentation container alongside the mason jar used as the collection container.*

During operation, it is important that the gas collection container is charged with ½ volume of water to allow the gas to dissolve and prevent dangerous pressure build up. The reactor is wrapped in aluminum foil to prevent contamination of the reactor by phototrophic organisms. For insulation we use a Styrofoam container that would further block photosynthetic organisms while increasing insulation and maintaining a tighter temperature distribution. Since the goal of the process being considered was to produce methane, it is important that the optimal conditions of methanogenesis be realized. Beneath the reactor is a hot plate set to roughly 40 degrees Celsius to maintain necessary temperature to allow for maximum efficiency[3]. Multiple sensors are placed atop the digester lid including a temperature, and barometric pressure sensor. A pH sensor is suspended inside of the digester to record fluctuations.

Arduino Data Collection

An Arduino Uno R3 development board was obtained along with the following sensors/attachments: *BME280 Pressure, Temperature, and Humidity Sensor* (Adafruit), *Analog PH Sensor/Meter Kit V2* (DFRobot), and *Adafruit Assembled Data Logging shield for Arduino* (Adafruit). The BME280 sensor measures pressure in hectopascals (1 hPa = 100 Pa), temperature in Celsius, humidity in percentage, and is able to measure altitude in meters. The two sensors were interfaced with the Arduino Uno using the I2C format (Figure 3) found at each respective sensor website[4, 5]. The sensor and attachment libraries for the Arduino IDE were obtained on GitHub (see links below). For each respective sensor, the example scripts *(bme280test* and *DFRobot_PH_Test*)*,* found in each library, were run to ensure the sensors were working properly.

Calibration of the pH sensor was done using MATLAB (Arduino Hardware Package), as the readability of MATLAB is greater than that of the Arduino IDE[6]. First, the output voltages of known pH's (4, 7, and 10) were measured five times each. Then, the MATLAB *polyfit(x, y, N)* function was applied to the voltage reading (*x*) and known pH values *(y)* using *N* values of 1 – 3. R values were calculated for each respective *N* value to determine the best fit; in this case it was linear. The linear pH equation based on voltage output was calculated and applied to the Arduino IDE example script. A new Arduino setup and script (*ReadBMEpH*) was generated to include both sensors (combining Figure 3 A and B) to ensure measurements could occur simultaneously.

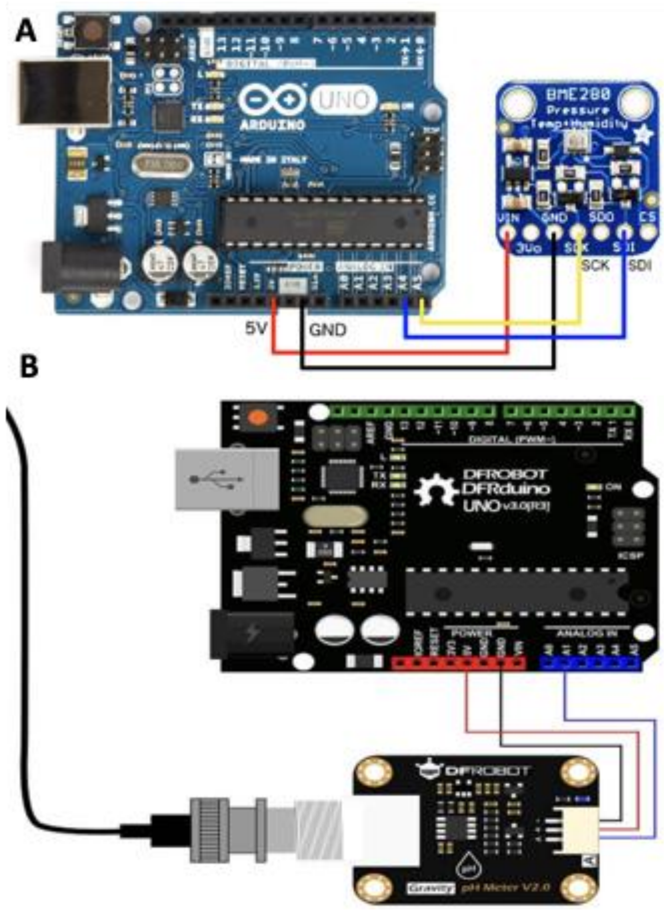

Figure 2: A. *BME 280 wiring diagram (3.3V input was used instead of 5V). Figure obtained from [7].* B. *pH sensor wiring diagram. (*Note: only one Arduino was used, and the two wirings were combined) Figure obtained from [8].*

The Data Logger, which came with a 2 GB SD card, was then attached to the Arduino (Figure 3 A) through solderless pins. The *CardInfo* script of the SD package (included with Arduino) was run to determine if the formatted SD card was supported (FAT16 or FAT32). Additionally, the real time clock (RTC) library was downloaded from GitHub so that measurements could be mapped back to a day and time. The RTC chip was located on the Data Logger (Figure 3 B) and the respective example script was deployed (*pcf8523* of the RTC package) to ensure accurate timing[10]. The BME280 and pH sensors were attached to the Data Logger with respective pins. The sensor Data Logger code, *LogBMEpH*, was written by following the Data Logger example script *lighttemplogger* (see link below). This example script was used as skeleton code, and the BME280 and pH sensors replaced their light and temperature sensors.

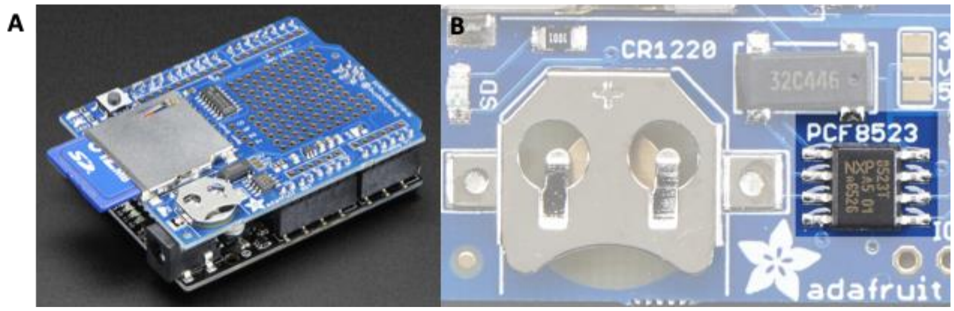

Figure 3: A. *Adafruit Assembled Data Logging shield for Arduino (top) attached to Arduino (bottom).* B. *RTC chip location (varies in different models of Data Logger). Figures obtained from [9].*

The software was written such that measurements would be logged every 10 minutes and saved to the SD card in CSV format. A new CSV file is written every two days containing with following columns: Millis, Datetime, Temperature (C), Pressure (hPa), Altitude (m), Humidity (%), pH; where Millis is milliseconds since the Arduino started, Datetime is the date and time of the recording, and the rest are measurements from the sensors. After each measurement is taken and written to the CSV file, the current CSV file is saved to ensure that large amounts of data are not lost. Data will be collected by an SD card reader every 5-7 days for analysis.

NOTE: GitHub Repositories Referenced in the Appendix

Mathematical Modeling

To predict the efficiency of the anaerobic digestion process that we are designing, we have developed a kinetic model that was adapted from Gebremedhin et. al[11]. The kinetic model was developed using MATLAB to create a code that allows for robust simulation of anaerobic digestion under different operating conditions. Some variables that can be analyzed through this program include feed stock composition, biodigester reactor volume, kinetic rate constant, feedstock mass and solid percentage etc.

The kinetic model utilizes some assumptions made by Gebremedhin et. al [11] to create effective approximations of biogas production under the simplified conditions. The primary assumption involved in the model is that digestion of solid waste into renewable biofuel occurs via a one step process:

$$C_nH_aO_b + (n - \frac{a}{4} - \frac{b}{2})\, H_2O \rightarrow \left(\frac{n}{2} - \frac{a}{8} + \frac{b}{4}\right) CH_4 + \left(\frac{n}{2} + \frac{a}{8} - \frac{b}{4}\right) CO_2 \quad (1)$$

where $C_nH_aO_b$ represents the complex organic matter in the feedstock and n, a, and b are dimensionless coefficients representing the atomic makeup of the organic feedstock. Additional assumptions in the development of this kinetic model include the following:

- Batch operation, no flow of material in or out of the anaerobic digester
- Fluid velocity is very low (negligible)
- Reactor is assumed to be adiabatic (well-insulated)
- Sludge is considered to be a Newtonian Fluid
- Temperature is considered as a constant variable
- pH is in mesophilic range
- Reaction is a one-step process
- Ignoring effect of vapor-liquid equilibrium (assuming single phase transport)
- Solution and vapor phase are assumed to be under ideal conditions

The kinetics of this expression can then be represented by the Arrhenius rate equation:

$$R_i = k_f\ C_i \sum [Reactants]^{C_i} \tag{2}$$

where k_f represents the kinetic rate constant of the forward reaction and C_i represents the numerical coefficient of the species of interest and C_j represents the numerical coefficient of the reactant in the rate expression. The quantity R_i is the molar rate of change of a particular species and for this anaerobic digestion model can be expressed by the following system of equations:

$$\frac{d[C_nH_aO_b]}{dt} = -k_f[C_nH_aO_b][H_2O]^{(n-\frac{a}{4}-\frac{b}{2})} \tag{3}$$

$$\frac{d[H_2O]}{dt} = -\left(n - \frac{a}{4} - \frac{b}{2}\right) k_f[C_nH_aO_b][H_2O]^{(n-\frac{a}{4}-\frac{b}{2})} \tag{4}$$

$$\frac{d[CH_4]}{dt} = \left(\frac{n}{2} - \frac{a}{8} + \frac{b}{4}\right) k_f[C_nH_aO_b][H_2O]^{(n-\frac{a}{4}-\frac{b}{2})} \tag{5}$$

$$\frac{d[CO_2]}{dt} = \left(\frac{n}{2} + \frac{a}{8} - \frac{b}{4}\right) k_f[C_nH_aO_b][H_2O]^{(n-\frac{a}{4}-\frac{b}{2})} \tag{6}$$

Combining these expressions with the concentration of each species at a given time point, yields the solution for the concentration of each species as a function of time:

$$[C_nH_aO_b]_t = \frac{d[C_nH_aO_b]}{dt}_t + [C_nH_aO_b]_{t-1} \tag{7}$$

$$[H_2O]_t = \frac{d[H_2O]}{dt}_t + [H_2O]_{t-1} \tag{8}$$

$$[CH_4]_t = \frac{d[CH_4]}{dt}_t + [CH_4]_{t-1} \tag{9}$$

$$[CO_2]_t = \frac{d[CO_2]}{dt}_t + [CO_2]_{t-1} \tag{10}$$

Once the specifications of the anaerobic digester are inputted, the simulation can be run for a determined time scale. For the purpose of this project, simulations were run for a period of 14 days at increments of 1 second. This resulted in the generation of 1209600 data points for each simulation. Each data point represented the concentration of each species. Using the inputted reactor conditions, the concentrations can be converted into mass units using the ideal gas law:

$$g\ of\ CH_4 = [CH_4]\ x\ Reactor\ Volume \div 16.04\frac{g}{mol}$$

The obtained amounts represent the theoretical quantities of biogas produced under ideal conditions for the anaerobic digestion process. As mentioned previously, one of the underlying assumptions is that the reaction proceeds to completion. However, this is almost never realized in actual anaerobic digestion processes. For this model to yield useful results, it must be correlated to actual data obtained for different anaerobic processes. To do this, data was obtained from multiple sources and then fitted using a nonlinear least squares regression analysis. This allowed for the computation of a fitting factor, a scalar multiplier used to approximate the kinetics of a process under actual conditions in relation to the proposed conditions. This fitting factor can be used to describe the “yield” of the process in relationship to the predicted theoretical conditions:

$$yield = \frac{actual\ biogas\ production}{theoretical\ biogas\ production} = fitting\ factor$$

NOTE: The Github repository for the MATLAB code for the mathematical model can be found in the appendix.

Results and Discussion

Laboratory-Scale Anaerobic Digester Design

Although validation of the design remains unrealized, a laboratory scale anaerobic digester was designed and constructed for a cost of <$300 and in a period of roughly 3 weeks. The setup was evaluated using simple tests like performing a seal test and pressure sensitivity tests using the Arduino module. The design has proven to be simple and elegant, occupying a very small footprint. We hope to be able to evaluate the efficacy of the anaerobic digester setup in the fall of 2020.

Mathematical Modeling

To test and validate the mathematical model that we have developed, pressure data was obtained from two different sources, representing a small[12]- and large[13]-scale anaerobic digestion process. The pressure data was converted into mass values via equations of state and then fitted to the model prediction to obtain the yield of the process and validate the kinetic assumptions. Multiple plots were generated including the overall conversion of each species (Figure 4) and the comparison between the experimental and theoretical production of biogas consisting of methane and carbon dioxide (Figure 5). It was observed that the data was in strong agreement with the kinetic model, corresponding to an R^2 range of 0.94 - 0.95.

For the first dataset, a study conducted by Rea 2014[12], evaluated the efficiency of anaerobic digestion on food waste in 1L steel reaction vessels. Pressure data was recorded in response to charging the digester with 100g of food waste and 100g of water. Prior to operation, analysis of the food waste found the atomic composition of the waste to be 27.2% C, 3.7% H, and 23.1% O. Pressure data was then recorded for a series of days. The first analysis done was on the predicted overall change in mass of each species in the proposed kinetic models.

Table 1: Summary of Simulation Conditions (Data Set 1):

Reactor Volume	1L
Food Waste	100 g
Water	100 g
Food Waste Composition	27.2% C, 3.7% H, 23.1% O
Simulation Time	14 days

Table 1: *Conditions specified for the simulation results depicted in Figure 4. The inputted simulation conditions match the experimental conditions used to obtain the data set presented by Rea 2014*[12].

Inputting the reaction conditions described in Table 1 yielded the results show in Figure 4.

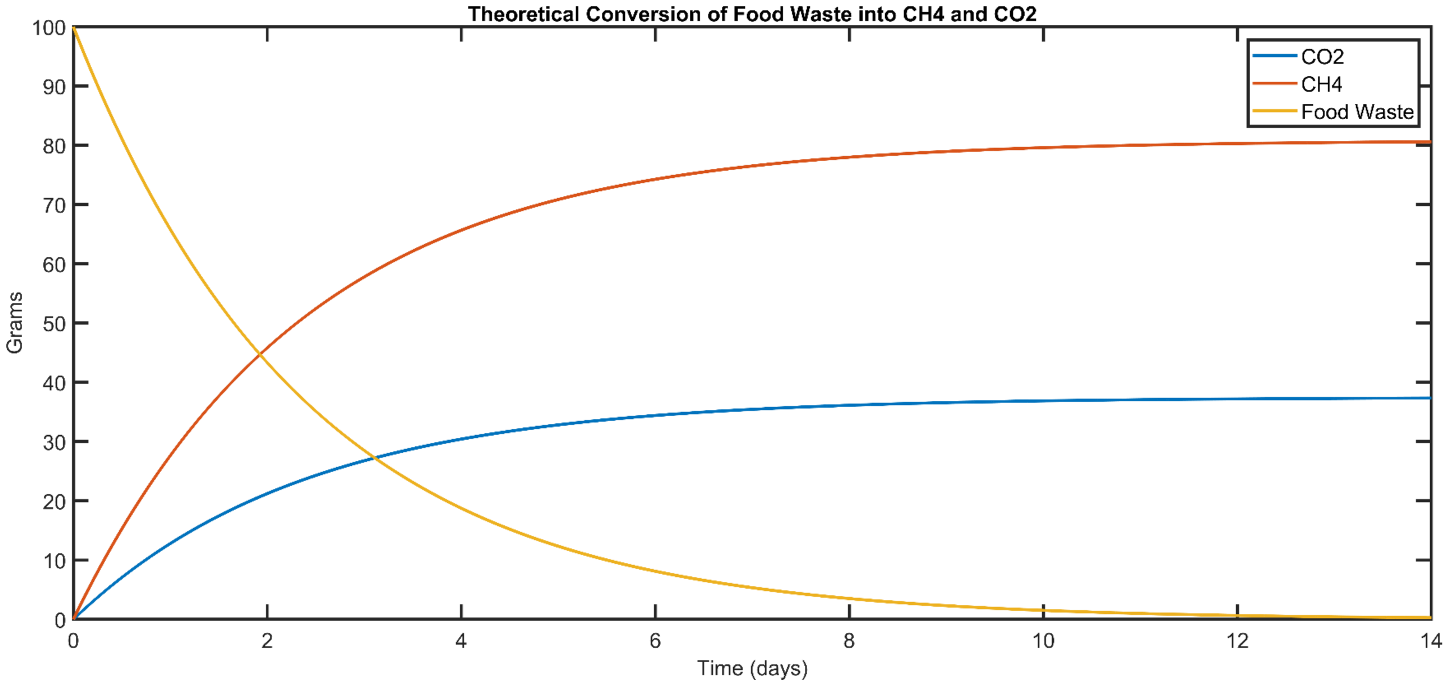

Figure 4: *Results of the simulation obtained for analysis of the conditions described by Rea[12]. The yellow curve depicts the depletion of the mass of the food waste over a period of 14 days, the blue curve depicts the accumulation of CO_2 over the period of 14 days, and the red curve depicts the accumulation of CH_4 over the period of 14 days. From the plot it appears that most of the biogas production is in the first 5 days, as typically observed in actual anaerobic digestion processes. Additionally, it is observed that under these ideal conditions almost all of the food waste is converted into biogas in a period of 14 days.*

Next, the pressure data obtained by Rea[12] was fitted to the model and the yield (fitting factor) was determined. To convert the pressure data into mass values, the ideal gas law was used with the assumption that the biogas produced is 70% CH_4 and 30% CO_2. The overall results of the fitting of the data can be found in Figure 5.

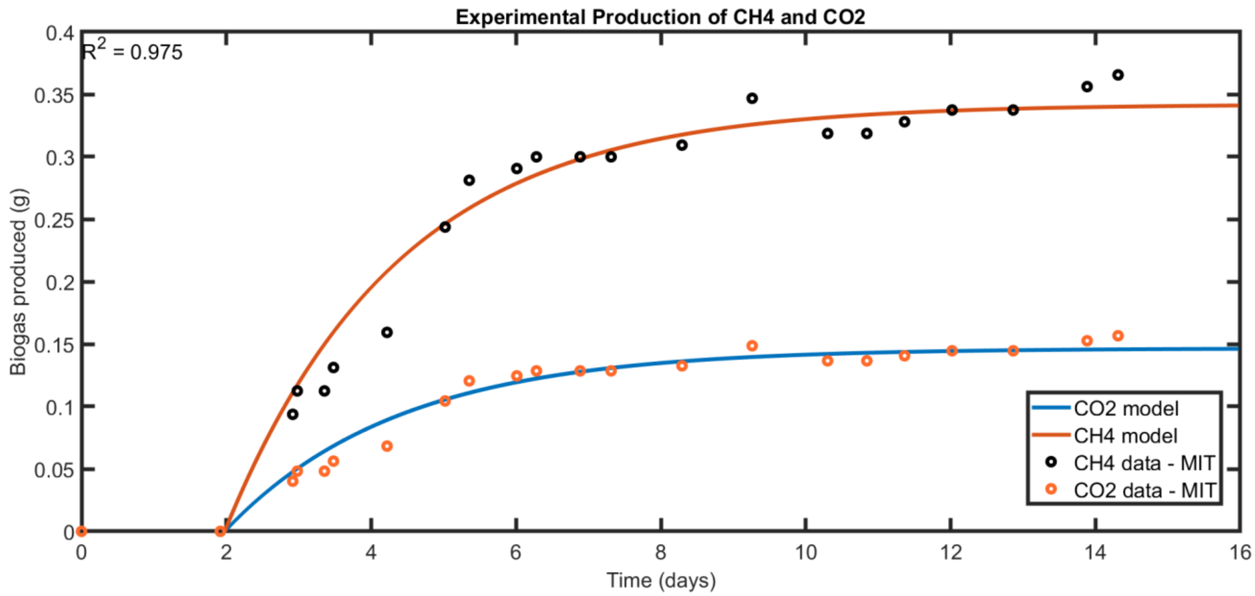

Figure 5: *Results of fitting the pressure data from Rea 2014[12] to the kinetic model. The data agrees quite well with the kinetic model and an R^2 of 0.945 was realized. The fitting factor was found to be 3.91×10^{-3}, representing the disparity between the actual and theoretical anaerobic digestion processes.*

Table 2: Summary of Results (Data Set 1):

	Predicted	Actual
Biogas Production	117.9 g	0.522 g
Percent Yield	100%	0.44%
R^2	1.0	0.945

Table 2: *Comparative summary of the results obtained by the simulation versus the actual experimental data. It can be observed that the yield of the simulation is much higher than the experimentally obtained value. Additionally, it appears that the trend of the simulation and experimentally obtained data agree quite well with an R^2 of 0.945.*

The same analysis was conducted using another data set obtained from Riggio et. al[13]. For this study, a larger scale anaerobic digestion process was analyzed by converting cow manure and whey mix into biogas. The reactor used in this process was a 128 L steel reactor. The waste that was charged into the reactor had an atomic composition of 66% nitrogen, 25% carbon, and 9% hydrogen. For this study, pressure data was measured over a period of 21 days after charging the reactor with 6 kg of waste and 16L of water. The analysis of this data set yielded very similar results to that of the first. It was observed that the data was in strong agreement with the kinetic model, corresponding to an R^2 of 0.951, and a fitting factor of 6.95 x 10^{-3}.The first step of the analysis was to analyze the predicted conversion of the solid waste into biogas. The results of the simulation with the conditions can be seen in figure 6.

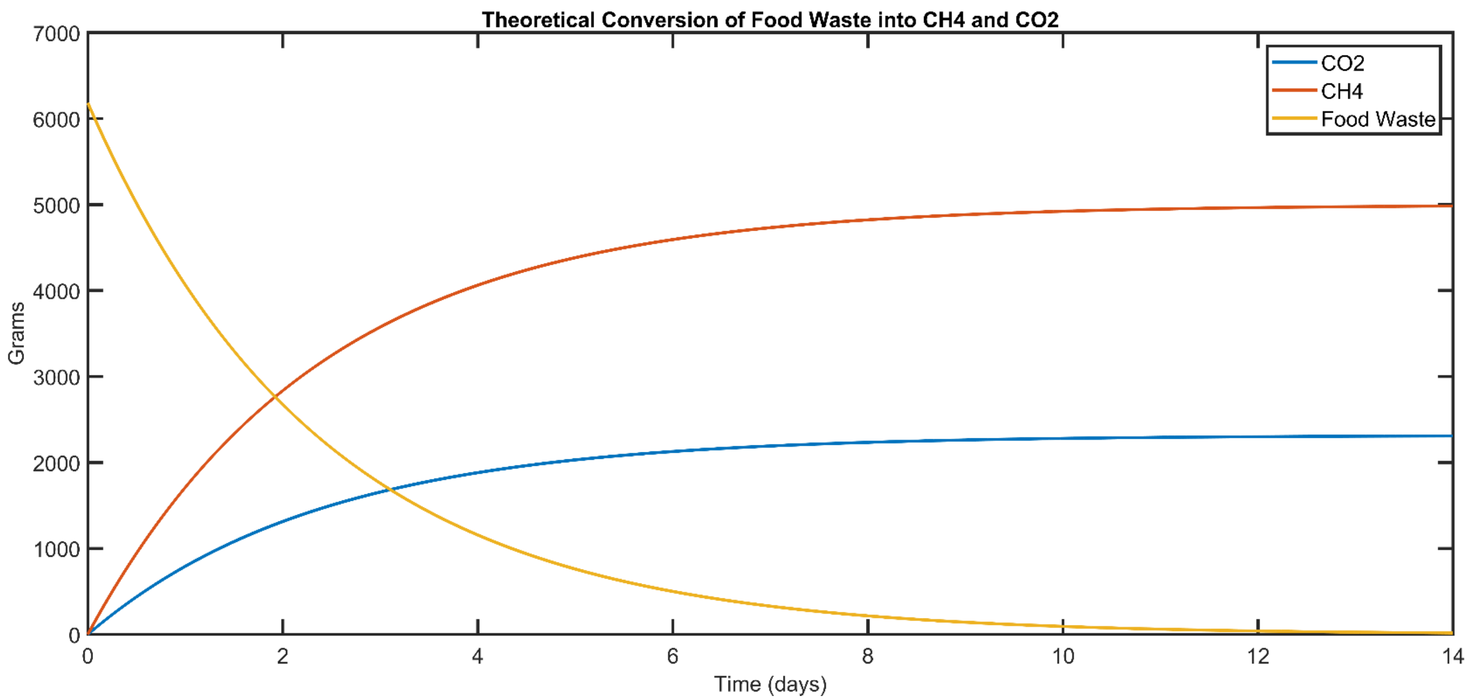

Figure 6: *Results of the simulation obtained for analysis of the conditions described in Riggio et. al[13]. The yellow curve depicts the depletion of the mass of the food waste over a period of 14 days, the blue curve depicts the accumulation of CO_2 over the period of 14 days, and the red curve depicts the accumulation of CH_4 over the period of 14 days. From the plot it appears that most of the biogas production is in the first 4 days, as typically observed in actual anaerobic digestion processes. Additionally, it is observed that under these ideal conditions almost all the food waste is converted into biogas in a period of 14 days.*

Next, the pressure data obtained by Riggio et. al[13] was fitted to the model and the yield (fitting factor) was determined. To convert the pressure data into mass values, the ideal gas law used with the assumption that the biogas produced is 70% CH_4 and 30% CO_2. The overall results of the fitting of the data using the experimental conditions found in table 3 can be found in Figure 8.

Table 3: Summary of Simulation Conditions (Data Set 2):

Reactor Volume	128L
Food Waste	6 kg
Water	16 kg
Food Waste Composition	66% N, 25% C, 9% H
Simulation Time	14 days

Table 3: *Conditions specified for the simulation results depicted in Figure 7. The inputted simulation conditions match the experimental conditions used to obtain the data set presented by Riggio et. al*[13].

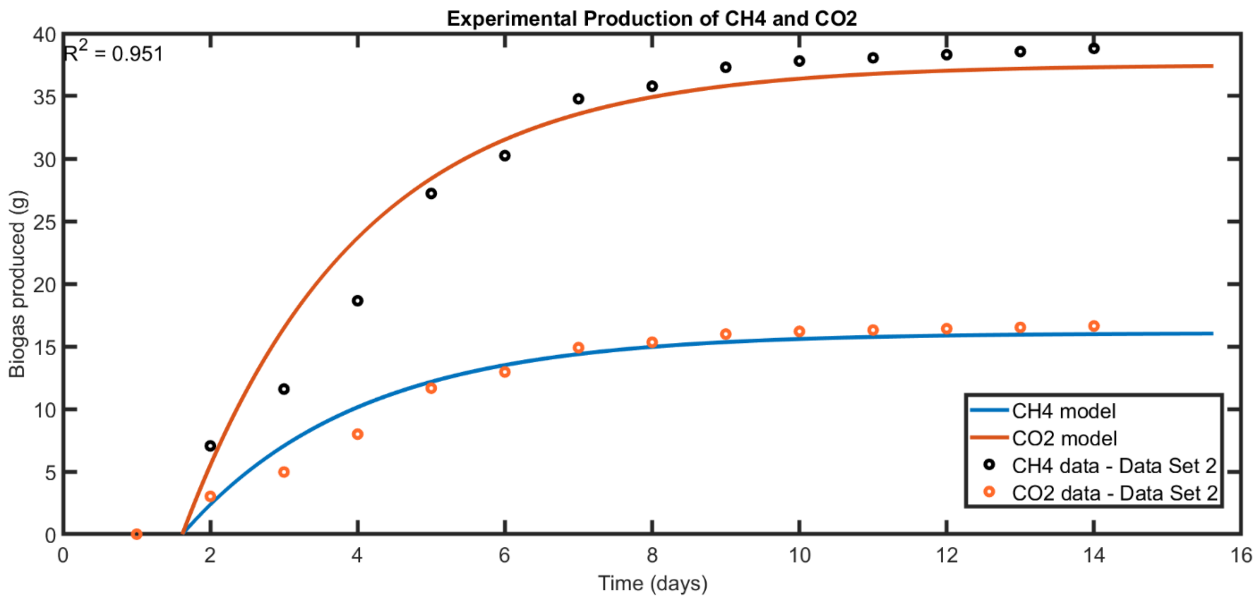

Figure 7: *Results of fitting the pressure data from Riggio et. al*[13] *to the kinetic model. The data agrees quite well with the kinetic model and an R^2 of 0.951 was realized. The fitting factor was found to be* 6.92×10^{-3}, *representing the disparity between the actual and theoretical anaerobic digestion processes.*

Table 4: Summary of Results (Data Set 2):

	Predicted	Actual
Biogas Production	7292.8 g	55.44 g
Percent Yield	100%	0.76%
R^2	1.0	0.951

Table 4: *Comparative summary of the results obtained by the simulation versus the actual experimental data. It can be observed that the yield of the simulation is much higher than the experimentally obtained value. Additionally, it appears that the trend of the simulation and experimentally obtained data agree quite well with an R^2 of 0.951.*

Analysis of both data sets yielded quite similar results. It was observed that the pressure data for various anaerobic digestion processes accurately followed that of the proposed kinetic model. Additionally, the yield was quite similar in magnitude for both processes. Using this information, additional data sets could be analyzed to determine the estimated yields for different anaerobic digestion feedstocks. This would allow for robust prediction of the yield of biogas produced under varying conditions. Future work for this model includes applying it to a larger range of materials and to increase the complexity to decrease the disparity between the actual and predicted biogas amounts. This would be accomplished by reducing the simplicity of the assumptions made and including complex mathematics into the framework from disciplines like heat and mass transfer, thermodynamics etc.

Conclusion

To develop tools to study anaerobic digestion on the laboratory scale, we developed a simple mathematical modeling using MATLAB that can be used to fit data to simulation results. This allows for the ability to determine the yield of a process in relationship to other processes and theoretical conditions. Additionally, we proposed the design of a small laboratory scale anaerobic digester that can be constructed for <$300 and in a period of less than 3 weeks. This laboratory scale anaerobic digester can be coupled with the simple mathematical model that we have developed in order to study the mechanisms underlying anaerobic digestion. Improvements in the fundamental understanding of the theory behind anaerobic digestion can result in improved reactor designs and the identification of conditions that improve the feasibility and efficiency of anaerobic digestion.

Additional Notes

Our work for the summer and fall periods of 2020 will be supported by a Sustainability Innovation Engagement Fund (SIEF) Grant valued at $2100. These funds will be used to purchase a pre-approved list of materials and hardware needed to construct the pilot-scale biodigester. Tentatively, if current circumstances with the COVID-19 situation make construction impossible, we will build off our math modeling work with advanced Aspen simulations

accounting for fluid thermodynamics and reaction engineering in our anaerobic digestion processes.

Appendix

Arduino GitHub Library Links:

- BME280 Library: https://github.com/adafruit/Adafruit_BME280_Library
- Analog pH Sensor Library: https://github.com/DFRobot/DFRobot_PH
- Adafruit Unified Sensor Library: https://github.com/adafruit/Adafruit_Sensor
    - Needed for any Adafruit sensor
- RTC library: https://github.com/adafruit/RTClib
- Data Logger Example (*lighttemplogger*): https://github.com/adafruit/Light-and-Temp-logger

Mathematical Modeling MATLAB Codes:

- anaerobicdigester.m: https://github.com/joshmcgee24/anaerobicdigester/blob/master/anaerobicdigester.m

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