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OPTIMIZATION OF BIOGAS PRODUCTION FROM *PHRAGMITES AUSTRALIS* USING FIRST-ORDER KINETIC MODELS

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Abstract. This study investigates the viability of *Phragmites australis*, commonly known as the common reed, as a sustainable feedstock for biogas production, emphasizing the effectiveness of pretreatment techniques to enhance biogas production. Given the invasive nature of *Phragmites australis*, the utilization of its biomass not only addresses environmental management challenges but also contributes to renewable energy solutions. The key objective is to evaluate mechanical and thermal pretreatment techniques on the anaerobic digestion performance of *Phragmites australis* using the first-order kinetic model biogas' cumulative production and volatile solids (VS) degradation were estimated. Sensitivity analysis was used to assess how different degradation rate constants and final biogas yield affected the efficiency of biogas generation. The degradation of VS was significantly accelerated by higher temperatures and finer particle sizes. Results indicate that both mechanical and thermal pretreatment significantly enhance biogas yield and degradation rates, milling (<1 cm) and moderate thermal treatment (100 °C, 2 h) providing optimal results. These studies highlight that the selection of appropriate pretreatment methods should be based on their sustainability and effectiveness in terms of reducing energy consumption and environmental impact.

Keywords: anaerobic digestion, biogas, pretreatment, *Phragmites australis*, kinetics.

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1. Introduction

As the demand for clean and sustainable energy sources increases, implementing waste-to-energy technologies has attracted significant attention. Waste management approaches are considered to effectively utilize the energy potential and simultaneously address waste disposal issues. Today, landfilling and incineration remain the most common waste management methods, which contribute to emissions of hazardous pollutants and greenhouse gas (GHG) emissions that threaten human and animal health. A widely adopted Waste-to-Energy (WTE) approach is the generation of biogas from organic-rich waste streams through the anaerobic digestion (AD) process (Bhatt & Tao, 2020). Promising and well-established mitigation options include harvesting and converting biomass into energy by producing biogas through AD. While anaerobic digestion lowers pollutants, it can also provide a source of energy through biogas (Arifan et al., 2021). Batch, plug flow, and total mix reactors are the three possible configurations for the AD process used to produce biogas, and each has advantages over the others. Batch reactors are becoming more common, most likely due to their ease of use and low construction cost, operation, and maintenance (Etuwe et al., 2016). The biogas production potential of *Phragmites australis* (*P. australis*) is significantly influenced by three primary factors: harvesting season, plant maturity, and pretreatment methods. Findings reveal that the optimal harvesting season for *P. australis* is between May and October. During this period, the plant exhibits higher nutrient content and lower lignin levels, increasing its digestibility and suitability for AD (Pelegrin & Holzem, 2017).

P. australis is a dominant plant species in wetlands across Lithuania and many other countries globally. It thrives in aquatic and wetland environments, forming dense stands along lake shores, riverbanks, and other wetland areas (Naugžemys et al., 2021). *P. australis* primarily consists of cellulose 38.13%, hemicellulose 20.51%, lignin 23.02%, extractives 6.90%, ash 4.25%, acetyl 3.92% and other 3.28%. Based on this information, *P. australis* has a very high organic content, making it a promising feedstock for biogas production. The presence of lignin inhibits enzymatic hydrolysis, necessitating effective pretreatment techniques (Gelosia et al., 2017).

Utilizing *P. australis* for biogas production presents some advantages, e.g., it naturally absorbs excess nutrients as they grow, which helps reduce overfertilization in marine ecosystems. Wet plant biomass makes them a renewable energy source and a potential solution for mitigating eutrophication. In this growing global issue, excessive nutrients in coastal waters lead to harmful algal blooms and oxygen depletion. As concerns over marine pollution rise, interest in these organic materials for sustainable energy continues to grow (Clifford, 2021). However, the main disadvantages include the prolonged time required for the process, sensitivity to temperature and pH fluctuations, and the potential release of GHG that contributes to climate change (Duan et al., 2025). Moreover, wet plants are a problem in numerous places because they contribute to clogging and overgrowth of water systems and decrease the use of an area for recreational purposes (Hansson & Fredriksson, 2004).

Temperature, retention time, Carbon/Nitrogen (C/N) ratio, organic loading rate (OLR), and pH are key operational parameters in the AD process (Uddin & Wright, 2023). Anaerobic digestion is a multifaceted biochemical process that is highly temperature-dependent, with fluctuations in temperature having the potential to impact both system efficiency and biogas output negatively. Temperature is a critical factor in modulating the metabolic functions of the microbial populations, which are responsible for breaking down organic material. Studies have demonstrated that biogas production is most efficient within specific temperature ranges, particularly between 28 °C and 35 °C (mesophilic conditions), where microbial activity reaches peak process stability and lower energy requirements (Anika et al., 2019) conditions, microbial performance declines, reducing biogas generation. For example, research highlights that operating outside the mesophilic range can significantly impair bacterial metabolic processes, reducing gas production rates. Thermophilic conditions where the temperature reaches 55–60 °C can lead to higher reaction rates and pathogen reduction but less stable. Temperature affects microbial growth rates, enzyme activity, and substrate solubility (Guo & Wang, 2024; Makaj Yai Chol et al., 2022).

The overall process's optimal pH range is typically from 6.5 to 8.0. Hydrolytic and acidogenic bacteria prefer pH between 5.5 and 6.5. Methanogens are sensitive to pH, with optimal growth around pH 7.0–8.0. pH affects microbial activity, substrate solubility, and the equilibrium of essential compounds. For the optimal development of methanogens, the C:N ratio should remain in the range of 20:1 to 30:1. The ratio parameter essentially reflects the concentration of easily biodegradable organic matter in the digestion substrate, a critical factor determining the efficiency of the process (Roj-Rojewski et al., 2019). These factors significantly affect the microbial communities responsible for the breakdown of organic matter and subsequent biogas production. Thus, understanding and optimizing these parameters is essential for maximizing biogas yield and ensuring process stability (Murillo-Roos et al., 2022).

A mathematical model is necessary to account for the effects of different mixing ratios of other feedstocks, substrate selection process, and loading rates and reduce energy and time during anaerobic co-digestion. These models are needed to predict performance, optimize, and prevent process instability and failure. Kinetic models can effectively understand the anaerobic digestion process and facilitate a deeper understanding of the complex biological processes involved in AD, enabling researchers to predict system behavior under varying operational conditions and to develop effective optimization strategies (Yu & Wensel, 2013). The main distinction between modeling with kinetic models and software as an anaerobic process (AP) and Anaerobic Digestion Model No. 1 (ADM1), is the degree of detail, the complexity of the models, and the program's computing power and flexibility which provide a wider scope for modeling complex biochemical processes, including Anaerobic Co-Digestion (AcoD) processes, while taking into account a wide range of parameters outside kinetics, whereas kinetic models concentrate on the comprehensive depiction of reaction kinetics in specific systems (Anukam et al., 2019). Kinetic models describe the relationship between substrate concentration, microbial growth rate, and product formation, which are valuable for understanding how changes in substrate availability affect microbial activity and biogas production rates. The predictive power of these models provides insight into the optimal conditions for microbial growth, which can be used to predict the performance of AD systems under various operational scenarios (Paramaguru et al., 2017). The first-order kinetic model is preferred because of its reliability, simplicity, and wide range of applications (Peng et al., 2024). Several mathematical models are commonly employed in modeling biogas production from *P. australis*. The modified Gompertz model is widely used to describe the cumulative biogas production over time, accounting for the lag phase, production rate, and maximum production potential, which is particularly effective for batch anaerobic digestion.

The modified Gompertz model:

$$Y_t = A \cdot exp(-exp\left(\left(\frac{R_{max} \cdot e}{A}\left(\lambda - t\right) + 1\right)\right), \tag{1}$$

where: Y_t – the cumulative biogas yield (mL/g) at time t (days); A – maximum biogas yield (mL/g); R_{max} – the maximum biogas production rate (day^{-1}); λ – lag phase (day); e – Euler's number (2.718282) (Tian et al., 2020). The Gompertz model solution methods are based on MATLAB, Microsoft Excel, Origin, SigmaPlot, and GraphPad Prism software platforms. Origin, SigmaPlot, and GraphPad Prism offer user-friendly interfaces and efficient workflows for curve fitting and graph visualization but often require carefully chosen initial parameter values to optimize model fitting effectively. Among other platforms, MATLAB has the advantage of being able to bypass the need to provide high-precision initial parameter values. However, the interface is not as user-friendly, and the operation itself is complex, with fitting and plotting requiring coding (Guo & Wang, 2024).

First-order kinetic models frequently quantify the rate at which VS degrades and the resulting methane generation. Although the first-order kinetic model is simple, widely applied for predicting biogas production from organic substrates, and requires minimal experimental data, it does not account for microbial adaptation phases, as seen in the Gompertz model, where a distinct lag phase is considered. The absence of a lag phase can result in the underestimation or overestimation of methane yield, particularly for substrates with complex degradation pathways (Kavan Kumar et al., 2023).

2. Method

The process shown in the diagram (see Figure 1) is systematic and involves the pretreatment of *P. australis* before being digested to produce biogas. The process is monitored through a data acquisition system, and the collected data is further analyzed through mathematical modeling to enhance efficiency and optimize conditions. The method includes a comparison of the biogas yield from *P. australis* under two mechanical and thermal pretreatments using the first-order kinetic equations (VS Degradation Model and Cumulative Biogas Production Model).

This section presents the layout and modeling of AD treatment from *P. australis* for biogas production, investigating the breakdown of volatile solids (VS) over time and the resulting biogas production. The process follows first-order kinetics, meaning that the rate of change is proportional to the remaining volatile solids. Methane yield is calculated using the VS Degradation Model and Cumulative Biogas Production. Based on the results provided by Gelosia et al. (2017) and Al-Iraqi et al. (2024), along with simulation data, 4.25% of the material is considered non-biodegradable ash and the initial VS content was determined as 95.75%, with a decay rate constant (k) of 0.05 day^{-1} and ultimate biogas production (B_0) of 78.21 mL CH_4/g VS.

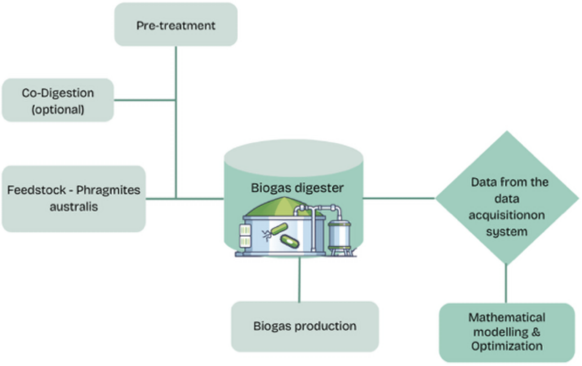

Figure 1. Optimization of biogas production process

First-Order Kinetics Models:
VS Degradation Model:

$$VS_t = VS_0 \cdot e^{-kt}, \tag{2}$$

where: VS_t – remaining volatile solids at time t; VS_0 – initial volatile solids; k – hydrolysis rate constant (day^{-1}); t – digestion time (days) (Huiliñir & Villegas, 2014)

Cumulative Biogas Production:

$$B_t = B_0 \cdot \left(1 - e^{-kt}\right), \tag{3}$$

where: B_t – the cumulative biogas yield (mL/g) at time t (day); B_0 – initial biogas yield; k – first-order decay rate constant (day^{-1}); t – digestion time (days) (Kavan Kumar et al., 2023).

Equations (2) and (3) help estimate the breakdown of organic material and the resulting biogas generation over time. Moreover, the effectiveness of pretreatment has been assessed by analyzing how different pretreatment conditions influence the degradation rate.

Table 1. Thermal and Mechanical pretreatment conditions of sensitivity analysis

Condition	Decay Constant (k) (day^{-1})	Ultimate Biogas Yield (B_0) (mL CH_4/g VS)
Untreated (5–10 cm)	0.05	78.21
Chopped (1–5 cm)	0.08	95
Milled (<1 cm)	0.12	105
Mild Thermal (70 °C, 1 h)	0.1	85
Moderate Thermal (100 °C, 2 h)	0.12	110
Severe Thermal (>120 °C, 4 h)	0.15	120

VS degradation and cumulative biogas production over 50 days were modeled using MATLAB to assess the effects of pretreatment conditions. The model included the impacts of mechanical pretreatment: size reduction as chopped (1–5 cm), milled (<1 cm, milling), and thermal pretreatment with varying retention periods and temperatures (70 °C, 100 °C, and >120 °C) as shown in Table 1.

3. Results and discussion

As shown in Figure 2 Volatile Solids (VS) Degradation over time where initially VS is 95.75%, but it decreases exponentially as the biomass is broken down. After 30 days, only ~21% of the initial VS remains, meaning most of the organic matter has already been degraded. The graph with Cumulative biogas production over time shows the amount of methane produced at 10 days about 31.84 mL CH_4/g VS is produced. By 30 days, the system has already produced ~80% of the total methane yield (62.5 mL CH_4/g VS), and by 50 days, the system is almost at the ultimate biogas production limit (78.21 mL CH_4/g VS).

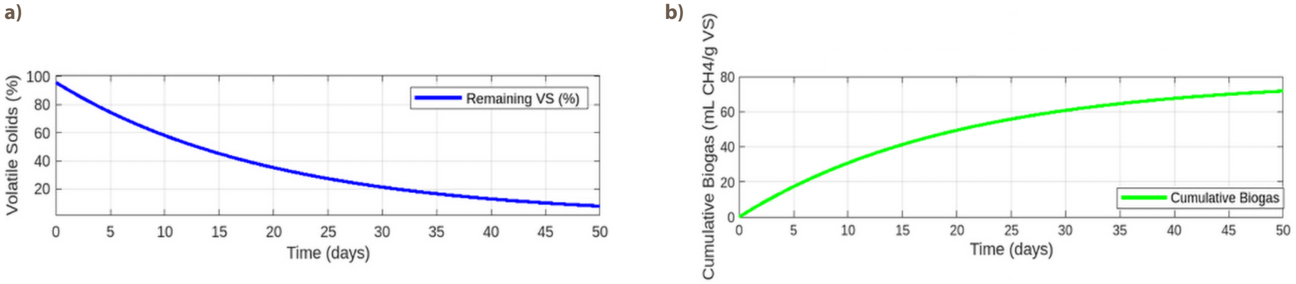

Figure 2. Results of first-order kinetic model for *P. australis* Anaerobic Digestion: a) Volatile Solids (VD) Degradation over time; b) Cumulative Biogas Production over time

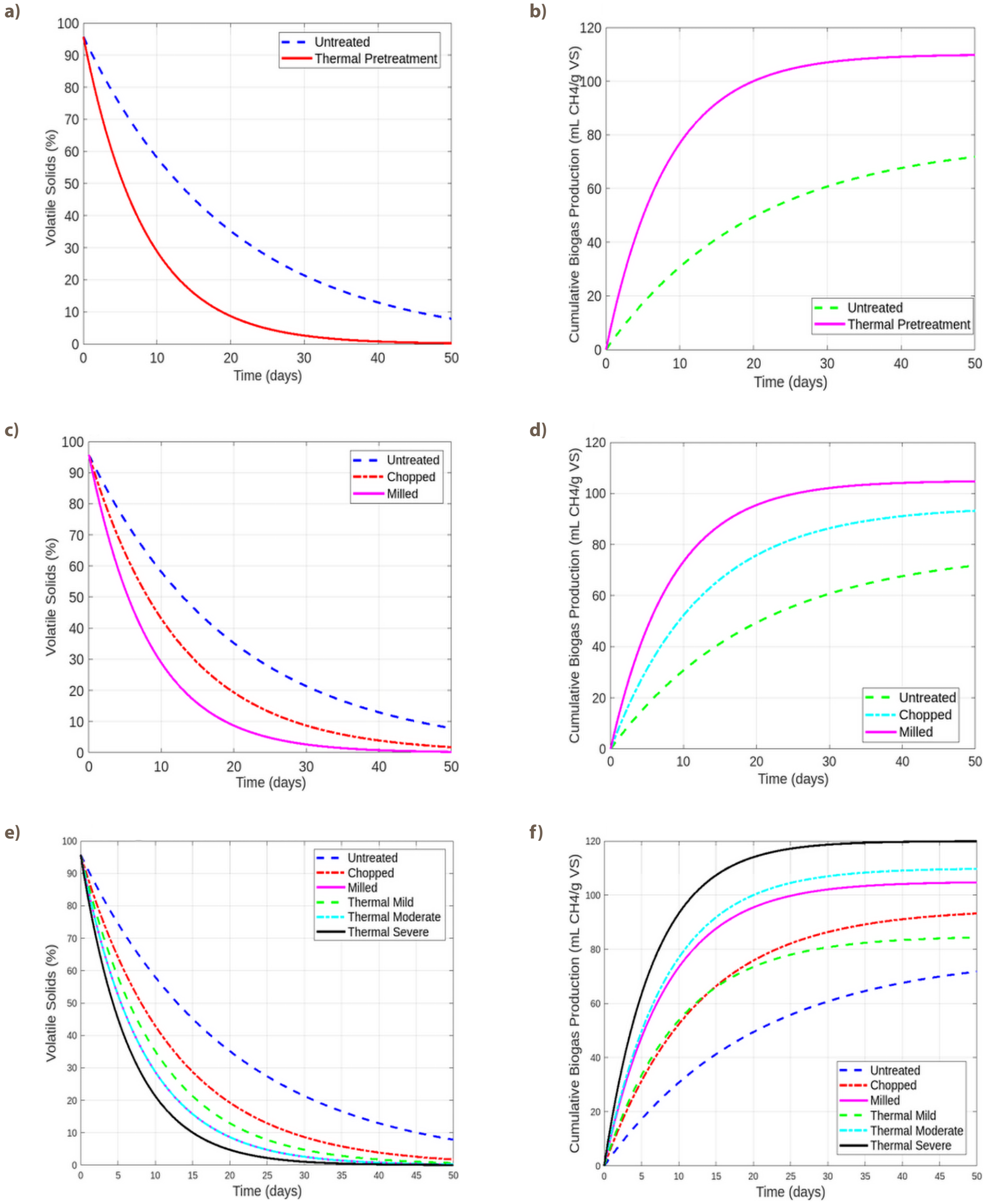

Figure 3. Results of first-order kinetic: a) VS Degradation: Untreated vs. Thermal pretreatment (pretreat); b) Biogas Production: Untreated vs. Thermal pretreat; c) VS Degradation: Untreated vs. Mechanical pretreat; d) Biogas Production: Untreated vs. Mechanical pretreat; e) VS Degradation: Mechanical vs. Thermal pretreat; f) Biogas Production: Untreated vs. Thermal pretreat

Sensitivity analysis helps assess how changes in key parameters (k, B_0) affect model outcomes, such as VS degradation and biogas production. While increasing led to higher methane outputs, higher values were associated with faster VS deterioration. First-order kinetics governs the process, which means that the rate of change is proportional to the number of volatile solids still present. The cumulative biogas production graph illustrated how higher temperatures and optimized milling improved methane output efficiency. Chopping and milling increase VS degradation rate k because smaller particles degrade faster but too fine milling (>500 μm) may not significantly improve results if considering energy costs.

The impact of thermal and mechanical pretreatment conditions on both VS degradation and cumulative biogas production is presented in Figure 3. Findings lead that the thermal pretreatment (>120 °C) produces the highest methane yield but risks degrading valuable fermentable matter. The results indicate that thermal pretreatment (100 °C, 2 h) and milling (<1 cm) provided the optimal balance between degradation efficiency and biogas production. While the untreated biomass had the slowest degradation and lowest biogas yield.

VS Degradation over time presents how organic matter decreases with time for different pretreatments. Cumulative Biogas Production over time shows how methane yield increases with time for the same pretreatment. These findings align with previous studies by Vasmara et al. (2023) and Al-Iraqi et al. (2024), which highlight the effectiveness of mechanical pretreatment in improving AD efficiency. Thus, particle size increases the surface area of biomass that is vulnerable to microbial attack, it can significantly affect the speed and stability of AD. According to the study, the overall quantity of biogas generated by the digestion of pre-treated *P. australis* varied considerably based on the size of the particles. Also, the analysis confirms that an optimal balance exists between degradation rate and biogas yield, ensuring efficient energy conversion without excessive substrate loss. Karthikeyan et al. (2024) provide insights that among the various pretreatment technologies, thermal pretreatment is effective, but it has high energy consumption and may produce hazardous waste. These statements confirm that severe thermal treatments (>120 °C) should be avoided unless energy recovery is optimized. Also, the increased energy consumption associated with mechanical and the use of expensive and caustic chemicals in chemical pretreatment technologies may negate the potential benefits of increasing biogas production, and precautions must be taken when handling hazardous chemical waste. Thus, careful assessment of sustainability, environmental impact, practicality, energy consumption, and scalability should be the foundation for choosing the most appropriate pretreatment technologies for anaerobic separation-based biogas production.

4. Conclusions

Phragmites australis has shown great potential as an energy source. This study confirms that mechanical and thermal pretreatment significantly improve the anaerobic digestion of *Phragmites australis*.

The choice of kinetic model for anaerobic digestion depends on the complexity of the substrate, microbial behavior, and process parameters influence.

Sensitivity analysis was conducted to evaluate the impact of varying degradation rate constants and ultimate biogas yield on biogas production efficiency. Higher values correlated with faster VS degradation, while increasing resulted in greater methane yields.

The first 20 to 30 days are the fastest for VS degradation and biogas production. After 30 days, most of the organic matter has decomposed and most biogas (~80%) is already produced.

Milling and moderate thermal treatment (100 °C, 2 h) were identified as optimal strategies, balancing biogas yield and process efficiency.

Thermal pretreatment (>120 °C, 4 h) was most effective for methane yield (120 mL CH_4/g VS).

Future research should explore combined pretreatments, economic feasibility analyses, and process optimization to enhance the biogas yield further.

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BIODUJŲ GAMYBOS IŠ *PHRAGMITES AUSTRALIS* OPTIMIZAVIMAS, TAIKANT PIRMOJO LAIPSNIO KINETINIUS MODELIUS

Z. Kazizova, A. Zagorskis

Santrauka

Šiame darbe tiriamas paprastosios nendrės *Phragmites australis* panaudojimas biodujų gamybai. Darbe vertinami optimalūs derliaus nuėmimo laikotarpiai bei veiksmingi pirminio apdorojimo metodai, siekiant maksimaliai padidinti metano išeigą. Atsižvelgiant į invazinį *Phragmites australis* pobūdį, jos biomasės naudojimas ne tik sprendžia su aplinkos taršos mažinimu susijusius iššūkius, bet ir prisideda prie atsinaujinančios energijos gamybos. Šiame tyrime taikomas pirmo laipsnio kinetinis metodas, siekiant ištirti mechaninio ir terminio apdorojimo poveikį *Phragmites australis* anaerobiniam apdorojimui. Taikant pirmo laipsnio kinetinį modelį buvo įvertinta kumuliatyvinė biodujų išeiga ir lakiųjų kietųjų dalelių (VS) skaidymas. Jautrumo analizė buvo įvertinta, kaip skirtingos skilimo greičio konstantos ir galutinis biodujų kiekis paveikė biodujų gamybos efektyvumą. Rezultatai rodo, kad tiek mechaninis, tiek terminis pirminis apdorojimas žymiai padidina biodujų išeigą ir VS skilimo greitį, o malimas ir vidutinis terminis apdorojimas (100 °C, 2 val.) užtikrina optimalius biodujų išeigos rezultatus.

Reikšminiai žodžiai: anaerobinis skaidymas, biodujos, pirminis apdorojimas, *Phragmites australis*, kinetika.