1. Background and Proposed Research

The world's growing population and rising energy demand have sparked renewed interest in renewable resources like biofuels, biochemicals, and biomaterials. Currently, fossil fuels are the main source of energy and are used to make various products, including synthetic polymers and cosmetics, that enhance our quality of life. However, the depletion of fossil fuel resources and their negative environmental impacts, such as greenhouse gas emissions, are driving the search for renewable alternatives. While fossil fuels have played a crucial role in global industrialization by meeting energy needs, their harmful effects are undeniable. Renewable energy sources like solar, wind, and geothermal can help generate electricity and heat, but they have limitations. Their availability can vary significantly due to seasonal or environmental changes, and importantly, they can't produce synthetic fuels for transportation[1]. They also face limitations in storage, energy density, and intermittency, which can hinder their ability to fully replace fossil fuels in the transportation sector.

A promising alternative to this challenge lies the utilization of lignocellulosic biomass for biofuels and green chemical production. Biomass, referring to living organisms excluding fossil fuels, serves as a renewable resource for fuel production[1]. Lignocellulosic biomass specifically comprised of cellulose, hemicellulose, and lignin offers a promising solution for biofuels production[2]. This biomass is inherently carbon-neutral; the CO_2 released during biofuel combustion is counterbalanced by the CO_2 captured during the plants' growth, contributing to the reduction of greenhouse gas emissions when compared to fossil fuels. Additionally, the utilization of lignocellulosic biomass supports waste management strategies by valorizing residues that would otherwise contribute to environmental pollution [2,3]. Its conversion to biofuels through technological advancements offers the potential for high efficiency and lower production costs over time, making it economically viable. Furthermore, the development of biofuels from lignocellulosic biomass can stimulate rural economies by creating new markets and job opportunities in biomass production, collection, and processing. Collectively, these advantages highlight the pivotal role of lignocellulosic biomass in shaping a sustainable, environmentally friendly, and economically beneficial energy future.

Lignocellulosic biomass, consisting of lignin, cellulose, and hemicellulose, is a renewable resource that holds great potential for the production of biofuels and bioproducts. They can be classified into several categories including agricultural waste, woody biomass, forest residue, and municipal waste. It should be noted that the complex and recalcitrant structure of lignocellulosic biomass poses significant challenges for microbial and enzymatic access to the fermentable sugars locked within cellulose and hemicellulose[2]. Pretreatment is therefore essential to alter the biomass structure, reduce its recalcitrance, and increase the accessibility of cellulose and hemicellulose for subsequent enzymatic hydrolysis. This process involves the use of physical, chemical, or biological methods to break down the lignin barrier, disrupt the crystalline structure of cellulose, and increase the porosity of the biomass. Without effective pretreatment, the conversion efficiency of lignocellulosic biomass into biofuels and other valuable chemicals would be severely limited, hindering the economic viability and sustainability of bio-based industries. Thus, lignocellulosic biomass pretreatment is a critical step in the bioconversion process, facilitating the efficient and cost-effective production of renewable energy and materials.

The primary objective of physical pretreatment is to reduce particle size, a goal attainable through various processes such as grinding, milling, or mechanical extrusion. However, physical processes are energy intensive and can incur higher costs compared to the final product [2].

Additionally, physical pretreatment may fall short in fully breaking down the complex structure of lignocellulosic biomass and often needs to be combined with other processes to achieve the optimal result [2]. ON the contrary, biological pretreatments utilize wood-degrading microorganisms to alter the chemical composition and/or structure of lignocellulosic biomass [3]. This modification enhances the biomass's suitability for enzyme digestion. The process entails minimal energy input and relies on incubating the biomass with specific microorganisms [4]. They are generally environmentally friendly and nontoxic. However, the primary concern with this technology is its low efficiency, how much it is affected by physical properties and long retention times [5].

Chemical pretreatment involves the application of an acid or base to lignocellulosic biomass, with the choice of chemical agent specifically influencing the breakdown of its various components. This method offers a targeted approach to pretreatment, enabling precise control over the degradation process and enhancing the quality of the final product. Chemical pretreatment proves especially effective in dismantling lignin, a complex and recalcitrant component of the biomass that is notoriously difficult to convert into value-added products. Despite its effectiveness, it's critical to acknowledge that chemical pretreatment processes can incur significant costs and pose environmental risks due to the use of harsh chemicals and the generation of hazardous waste [6]. In contrast, oxidative pretreatment involves the introduction of oxidative agents to the biomass like ozone to initiate chemical reactions and modify the structure of the biomass. It breaks down lignin and separates the cellulose crystals [6]. Ozone reacts preferably with lignin than carbohydrates. Because of this preference for lignin using ozone leads to a more efficient release of sugars during enzymatic hydrolysis [7]. Additionally, ozone can be used to selectively transform lignin to high value-added platform compounds [8]. Ozone's application for pretreatment could minimize the need for harsh chemicals that are expensive and pose severe environmental risk [9]. Nevertheless, ozone production can be energy-intensive and poses potential health risks upon close contact. Despite these challenges, ozone presents similar benefits to chemical pretreatment, including a reduced environmental impact and lower chemical costs.

Several studies have explored the use of ozone for biomass pretreatment (ozonolysis process) [10 – 12]. One study used ozone for rice husk pretreatment, increasing methane production by 42% [10]. Another study used ozone on sugarcane straw pretreatment, resulting in a 75% boost in cellulose and a 42% increase in hemicellulose, with a decrease of 47% in lignin content [11]. The higher cellulose and hemicellulose levels suggest better access to fermentable sugars, crucial for biofuel production. Ozone has proven effective in pretreatment, but there's a gap in research focusing on detailed economic and environmental assessment of ozone utilization for biomass pretreatment and subsequent conversion to biogas via anaerobic digestion. Furthermore, it is not clear how the properties of biomass could influence the ability of ozone to effectively delignify biomass materials. To fill this research gap, the following objectives are proposed.

Research Objectives:

- **Research objective 1 (RO1):** This objective aims to comprehensively assess how different properties of biomass, such as composition, density, and moisture content, affect the efficiency of ozone delignification. Understanding these relationships is crucial for optimizing the pretreatment process to achieve maximum delignification with minimal damage to the cellulose content.
- **Research Objective 2 (RO2):** Using insights from RO1, this objective focuses on creating an accurate and reliable process simulation model that reflects the real-world

operation of ozone pretreatment. This model will be used to conduct a thorough economic analysis, assessing the cost-effectiveness of ozone pretreatment compared to traditional methods. Additionally, an environmental impact assessment will be performed to evaluate the sustainability of implementing ozone pretreatment in biomass processing, considering factors such as energy consumption, greenhouse gas emissions, and potential pollution.

Hypothesis:

- It is hypothesized that a detailed comprehension of how biomass properties affect ozone delignification will lead to optimized pretreatment conditions, enhancing biomass conversion processes' efficiency and sustainability.

2. Methodology

The proposed project's methodology and research plan unfold in two sequential work phases. In Phase 1, emphasis will be on performing a detailed literature review and compiling data related to biomass properties (proximate, ultimate, and compositional analysis) and delignification percent. The compiled data will be used to develop a process simulation model using Aspen Plus. Aspen Plus is a comprehensive process modeling software used for the simulation and optimization of chemical processes in industries such as chemicals, pharmaceuticals, and energy, enabling engineers to evaluate and improve plant performance and efficiency. Following the process simulation, a sensitivity analysis will be performed to understand how changing biomass influences the delignification effectiveness.

In subsequent work, a detailed techno-economic and environmental assessment of the two processes will be performed. The Aspen Plus Economic Analyzer will determine equipment purchase costs, while discounted cash flow analysis will appraise the cost of ozone pretreatment.

The second phase will focus on the environmental assessment of ozone pretreatment and its comparison with other pretreatment methods. OpenLCA software, along with process simulation data in phase 1, will be utilized for environmental impact assessment. Through the OpenLCA the greenhouse gas emissions as well as the human toxicity and freshwater toxicity of ozone pretreatment will be evaluated.

3. Project timelines

The Gantt chart has been developed and presented in figure 1. The diagram illustrates the project milestones including two identified research objectives. Each objective is designed to be completed independently in two weeks. The following activities and deliverables planned for the 5 weeks duration are also documented in the Gantt Chart:

Data compilation: A comprehensive literature review will be conducted to collect the data required for process simulation during this work phase.

Final report submission (FR): A comprehensive report detailed the summary of research performed over the entire project duration.

Table 1: Gantt chart showing the project timelines and key research objectives.

May 31, 2024- July 30, 2024		

Week	1	2	3	4	5	6	7	8	9	10
Data compilation	ORS									
Research Objectives 1				RO1						
Research Objectives 2							RO2			
Monthly Reports				MR1			MR2			
Final Report								FR		

Conclusions

The expected outcome of this research is to establish a clear understanding of the impact of biomass properties on the efficiency of ozone delignification, leading to the optimization of the pretreatment process for enhanced biofuel production. By achieving Research Objective 1, we aim to identify the key biomass characteristics that significantly influence the delignification process, enabling the development of a more effective and less damaging pretreatment method. Subsequently, Research Objective 2 will leverage these insights to create a comprehensive process simulation model. This model will not only assess the economic viability of ozone pretreatment in comparison to conventional methods but will also evaluate its environmental sustainability by analyzing energy usage, greenhouse gas emissions, and potential pollutants. Ultimately, this research seeks to provide a scientifically grounded, economically sound, and environmentally friendly framework for the application of ozone pretreatment in the biomass-to-biofuel conversion process, potentially revolutionizing the biofuel industry by making it more sustainable and cost-effective.

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